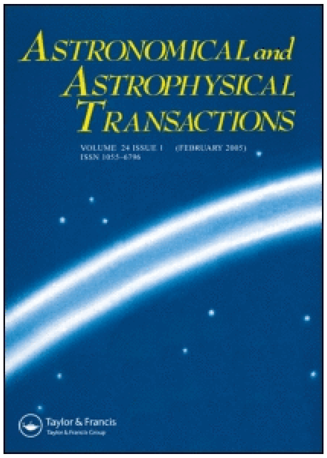

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Yu. N. Mishurov [a]
[a] Department of Astrophysics, Rostov State University, Rostov-on-Don, USSR

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GALACTIC DENSITY WAVES TRIGGER FORMATION OF H_2 MOLECULES

Yu. N. MISHUROV

Department of Astrophysics, Rostov State University, 5 Zorge, 344104, Rostov-on-Don, USSR

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The flow of interstellar gas in the gravitational field of galactic density waves has been investigated in the framework of the diffusion approximation with allowance for thermal processes and molecular hydrogen formation. The galactic density waves are shown to stimulate the formation of H_2 molecules. The proposed theory explains the existence of two displaced spiral arm systems discovered in M51 using different tracers, namely CO, dust and continuum, and also HI and H_α. The "atomic precursor" phenomenon, i.e., a narrow region of high HI density at the inner edge of the molecular arm is predicted.

KEY WORDS Galaxies, spiral-interstellar medium, molecules.

1. INTRODUCTION

Already in the 1970s, the idea was proposed that galactic density waves (GDW) and galactic shocks, which are responsible for formation of bright stars in the spiral arms, dust lanes at the inner edge of the arms, enhanced synchrotron radiation etc., trigger formation of molecules in the interstellar medium (ISM) (see, e.g., Burton, 1976). It was shown by Marochnik *et al.* (1983, hereafter MBMS) in the framework of microscopic description of the ISM (see Sect. 2 below) that a very strong wave arises in the inner part of Galaxy (at the galactocentric distance $\varpi \sim 5$ kpc) under the influence of the GDW. We called this the accretion wave (AW). The arguments in favor of the formation of molecular hydrogen under the influence of the AW can be found in Mishurov (1990). In fact, the critical density ($\sim 10^2$ cm^{-3}) required for hydrogen to transfer efficiently into the molecular phase (Hollenbach *et al.*, 1971, hereafter HWS) and a low temperature (~ 25 K), close to that observed in molecular clouds, are typical of the AW. Furthermore, the AW flow occurs in the region where there is a maximum in the H_2 distribution (such phenomenon does not take place at the solar galactocentric distance, see MBMS). However, the GDW influence on kinetics of H_2 formation has not been studied up to now. Our purpose here is a direct computation of the process.

In Sect. 2 the model is described and the basic equations are given. The results are presented in Sect. 3. In Sect. 4 we discuss general conclusions and compare our results with observations of M51 in CO($1 \rightarrow 0$) line (Vogel *et al.*, 1988, hereafter VKS), thermal, nonthermal and H_α emission (Tilanus *et al.*, 1988, hereafter TAHCK).

2. BASIC CONCEPTS AND EQUATIONS

We consider a model problem of perturbations generated in the ISM by the gravitational field of the GDW propagating in stellar disk while the gas flows through a spiral arm. Before writing equations, we specify the model of the ISM.

In a classical scheme of Roberts (1969), a phenomenological description of the medium properties has been used. Indeed, HI clouds are considered as gas "particles" and the ensemble of these particles is assumed to be isothermal. In our model, atoms and molecules are the medium particles themselves, and we take into consideration both thermal and chemical processes in the gas. It is quite natural to call such a description of the gas properties a "microscopic" one. Furthermore, we neglect the cloud structure of the ISM assuming that cloud matter is spread over the space and investigate the gas evolution in the diffuse approximation. In our opinion, the cloud structure of the ISM is very important but we restrict ourselves to the diffuse approximation to simplify calculations.

Now we turn to mathematical formulation of the problem and the corresponding equations. In the absence of the GDW, the galactic gravitational field is axisymmetric. In such a field, the gas motion is assumed to be circular at the angular velocity $\Omega(\varpi)$. Then a perturbation field from the GDW whose potential is φ_s is introduced. Our aim is to calculate perturbations in the gas induced by this field.

Equations of interstellar gas motion disturbed by the GDW gravitational field with allowance for thermal processes and H_2 molecule formation in a galaxy with a tightly wound spiral arms have the form (MBMS, Alexeev and Grishin, 1985):

$$\frac{d\rho}{dt} + \rho\frac{\partial u}{\partial \eta} = 0, \tag{1}$$

$$\frac{du}{dt} - 2\Omega(v - v_0) = -\frac{1}{\rho}\frac{\partial p}{\partial \eta} - \frac{\partial \varphi_s}{\partial \eta}, \tag{2}$$

$$\frac{dv}{dt} + \frac{æ^2}{2\Omega}(u - u_0) = 0, \tag{3}$$

$$\frac{d\eta}{dt} = u, \tag{4}$$

$$\frac{d\varepsilon}{dt} + \frac{p}{\rho}\frac{\partial u}{\partial \eta} = \Gamma - \Lambda, \tag{5}$$

$$\frac{dx_2}{dt} = 2R' n_d(1 - x_2) - \zeta_2 x_2, \tag{6}$$

$$\varphi_s = A\cos\left(\frac{2\eta}{\varpi \sin i}\right), \tag{7}$$

where u and v are the perpendicular and tangential to the arm gas velocity components measured in the reference frame rotating at the angular velocity of the spiral pattern Ω_p, $u_0 = \varpi(\Omega - \Omega_p)\sin i$ and $v_0 = \varpi(\Omega - \Omega_p)\cos i$ are their undisturbed values, i is the pitch angle, η and ζ are the distances across and along the arms, respectively (the WKB-approximation of tightly wound spirals, $i \ll 1$,

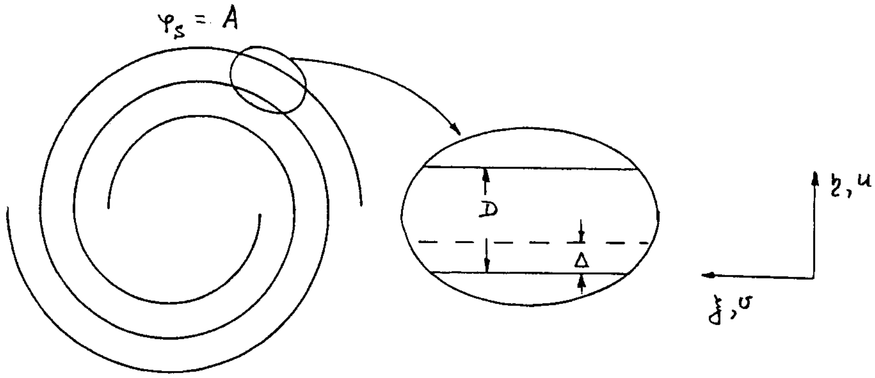

Figure 1 The view of a spiral galaxy from above. *Left*: the spatial structure of the φ_s level lines. *Center*: a closer view at the selected region. D is the distance between arms. Dashed line is the bright stars location. Δ is the distance between the bottom of the potential well of the GDW and the bright stars location. *Right*: the local Cartesian coordinates with the axes η (perpendicular to the arm) and ξ (parallel to the arm). $\Delta = 0{\cdot}5$ cpc.

means that the arms curvature can be neglected and all quantities vary mainly across the arms, that is $\partial/\partial\eta \gg \partial/\partial_\xi$, see Figure 1). Furthermore, ϖ is a slow coordinate and η is a fast coordinate; these should not be mixed with Roberts' spiral coordinate; ρ, P and ε are the density, pressure and specific (per unit mass) internal energy, t is time, Γ and Λ are the specific heating and cooling rates of the gas, R' is the H_2 formation rate; $n_d \approx 4 \cdot 10^{-13} \cdot n_H$ is the dust grains concentration, $n_H = n_1 + 2n_2$ is the total volume density of hydrogen atoms, n_1 and n_2 are the atomic and molecular hydrogen densities, $x_2 = 2n_2/n_1$ is the relative concentration of molecular hydrogen, ζ_2 is the dissociation rate of H_2, A is the spiral potential amplitude, and æ is the epicyclic frequency. The mass density of the gas mixture, ρ, is connected with the total number density n by $\rho = mn$, where $m = 2.16 \cdot 10^{-24}$ g is the average mass of a gas particle, $n = n_H + n_{He}$, and $n_{He} = 0.1\, n_H$ is the helium number density.

Thermodynamical equations should be added to this system:

$$\varepsilon = \frac{3}{2}\frac{p}{\rho}, \tag{8}$$

$$p = (n_1 + n_2 + n_{He} + n_e)\kappa T, \tag{9}$$

where T is the gas temperature, n_e is the electron density, κ is the Boltzmann constant.

In order to close the above system of equations it is necessary to specify thermal and ionization processes occuring in the medium (the chemical kinetics equation is given below). Let us discuss them briefly. The situation is more or less clear with the gas cooling (connected mainly with the atom exitation by inelastic collisions with free electrons and hydrogen atoms and consequent energy loss by radiation; expression for Λ is given by Penston, 1970 and Goldsmith *et al.*, 1969). However, heating and ionization processes are more complicated. The problem was discussed by many authors. Without going into details, we only mention that there are perhaps three regions in the Galaxy, where different mechanisms prevail: (*i*) the central region, $\varpi < 5$ kpc, where the main contribution to the heating and ionization is made by expanding supernova envelopes; (*ii*) the inner region, $5\,\text{kpc} \lesssim \varpi \lesssim 10$ kpc, where cosmic rays dominate and (*iii*) the outer region, $\varpi > 10$ kpc, where the impact of high velocity clouds makes a considerable contribution to the gas heating (see Heiles, 1987; Tenorio-Tagle *et al.*, 1986).

We pay special attention to the region close to the maximum in H_2 distribution within the galactic molecular ring ($\varpi \approx 5$–6 kpc). Thereby, we adopt subcosmic rays as the ionizing and heating agent. Expression for Γ is given by Goldsmith *et al.* (1969). The electron ionization degree $x_e = n_e/n_1$ can be found from the ionization equilibrium equation

$$x_e = (q^2 + 2q)^{1/2} - q,$$

where $q = \zeta_H/(2\alpha n_1)$, $\alpha(T)$ is the hydrogen recombination coefficient, and ζ_H is the hydrogen ionization rate.

It is obvious that ζ_H varies in space and time. Strictly speaking, one should consider equation for this quantity and calculate it while considering gas evolution. However, in a first approximation we restrict ourselves to a model with $\zeta_H = \text{const} \sim 10^{-15}\,\text{s}^{-1}$ ($\zeta_H = 9 \cdot 10^{-16}\,\text{s}^{-1}$ is assumed in calculations).

To conclude the discussion of thermal and ionization phenomena in the ISM, it is worth noticing that, as the first step, we restrict ourselves to the processes involving atomic hydrogen. The results obtained in our earlier papers provide some justification for this assumption. As noted in Introduction, even when effects associated with H_2 are neglected, the GDW result in very strong accretion wave in the discussed range of galactocentric distances. The gas density in the AW reaches the threshold for H_2 formation. Nevertheless, this does not exclude the necessity to consider the effects of molecular cooling.

Let us turn to kinetics of H_2 production and destruction. The main channel of H_2 formation in the ISM is the reactions on the surface of dust particles. The rate of this process is determined by the reaction constant $R = R' n_d/n_H$ in Eq. (6). The latter varies, in particular with the dust temperature. Again, we should have calculated the dust temperature in a self-consistent manner. However, to simplify the calculations we assumed a constant value $R = 2 \cdot 10^{-16}\,\text{cm}^3 \cdot \text{s}^{-1}$ (calculations with $R = 2 \cdot 10^{-17}\,\text{cm}^3 \cdot \text{s}^{-1}$ yield similar results; R can reach $\sim 10^{-15}\,\text{cm}^3\,\text{s}^{-1}$, see Smoluchowski, 1983).

Now we proceed to the H_2 dissociation. Molecules dissociation is caused by the ultraviolet radiation of bright stars. According to HWS, the H_2 dissociation rate is given by

$$\zeta_2 = G_0 \frac{\pi e^2}{m_e c} \sum_i k_i h_i f_i j_i, \tag{10}$$

where $G_0 \sim 10^{-8}$ photon $\cdot\,\text{cm}^{-2} \cdot \text{s}^{-1} \cdot \text{Hz}^{-1}$ is the ultraviolet photon flux in the wavelength range $\lambda \approx 912 - 1100$ Å, i.e., in the domain free from attenuation by dust or molecular clouds; j_i is the self-shielding function (Federman *et al.*, 1979; HWS). For other notation, see HWS. Summation (10) is carried over the lines of Lyman band.

An approximate expression for ζ_2 can be obtained the following way. We consider that photon absorption occurs in a single effective spectral line with the central wavelength $\lambda_c = 1000$ Å and with the width determined by the Doppler broadening due to thermal motion. Then (10) takes the form

$$\zeta_2 = \zeta_{20} j_{\text{eff}}, \tag{11}$$

where $\zeta_{20} \sim 10^{-10}\,\text{s}^{-1}$ (HWS), j_{eff} is the effective self-shielding function

$$j_{\text{eff}} = \frac{1}{G_0} \frac{\int G(\eta, \nu)\, d\nu}{\int \sigma(\nu)\, d\nu},$$

G is the photon flux at η, $\sigma(\nu)$ is the cross-section of the photon absorption, and ν is the frequency.

To calculate $G(\eta, \nu)$, we consider spiral arms as being tightly wound. As mentioned above, the arm curvature can be neglected in this approximation and the arms can be considered as planes parallel to each other and to the galactic axies of rotation (see Figure 1; recall that we have neglected the gas motion along the rotation axis). Having assumed that the stars are distributed uniformly along the planes and H_2 dissociation is taking place at the point η under the action of the closest arms between which this point resides, we obtain

$$G = \frac{G_0}{2}\left[\exp\left(-\int_{\Delta}^{\eta} æ_f\, d\eta'\right) + \exp\left(\int_{\Delta+D}^{\eta} æ_f\, d\eta'\right)\right],$$

where Δ is the distance from the φ_s minimum position to the plane on which bright stars are located, $D = \pi\varpi \sin i$ is the distance between the arms (see Figure 1), $æ_f = æ_d + æ_g$, $æ_d = \pi r_d^2 n_d$ is the coefficient of photon absorption by dust, $r_d \approx 1, 7 \times 10^{-5}$ cm is the average grain radius, $æ_g$ is the absorption coefficient due to molecular hydrogen.

Altogether, expression for j_{eff} can be written in the following form:

$$j_{\text{eff}} = \frac{1}{2}\left[j_1 \exp\left(-\int_{\Delta}^{\eta} æ_d\, d\eta'\right) + j_2 \exp\left(\int_{\Delta+D}^{\eta} æ_d\, d\eta'\right)\right],$$

where

$$j_{1,2} = \frac{1}{\sqrt{\pi}} \int_0^{\infty} \exp[-\vartheta^2 - \tau_{1,2}\exp(-\vartheta^2)]\, d\vartheta,$$

$$\tau_1 = \frac{\sqrt{\pi}\, e^2}{m_e c} \overline{hf} \int_{\Delta}^{\eta} \frac{n_2}{\beta}\, d\eta',$$

$$\tau_2 = \frac{\sqrt{\pi}\, e^2}{m_e c} \overline{hf} \int_{\Delta+D}^{\eta} \frac{n_2}{\beta}\, d\eta',$$

$\overline{hf} \approx 0.02$ (HWS), and $\beta = \lambda_c^{-1} (\kappa T/m_{\text{H}})^{1/2}$ is the Doppler width. We have used approximate formulas of Federman *et al.* (1979) for calculation of $j_{1,2}$.

The given relations complete the system of gas dynamics equations governing the ISM evolution in terms of the "microscopic" description. The boundary and initial conditions should be added to them. As the Boundary conditions, we take the periodicity of all gas dynamics quantities in η with the period D. Suppose that at the initial moment, $t = 0$, the GDW is absent ($\varphi_s = 0$) and all gas dynamics quantities are equal to their unperturbed values: $n = n_0$, $u = u_0$, $v = v_0$, and $T = T_0$ (T_0 follows from thermal balance condition $\Gamma(n_0, T_0) = \Lambda(n_0, T_0)$ for given n_0). In addition, we adopt $x_{20} = 0$.

The numerical method employed for solving the gas dynamics equations is similar to that suggested by Samarskii and Popov (1980).

We stress again that, for the sake of simplicity, we do not take into account such factors as thermal processes due to molecular hydrogen, the cloud structure of the ISM, etc. On the other hand, we shall be able to assess the role of each such factor by including it separately into the model.

3. RESULTS

To understand the role of the GDW in the chemical evolution of the gas and the formation of its large-scale structure, consider the initial state without the GDW ($\varphi_s = 0$). If we neglect the photon absorption ($æ_f = 0$), Eq. (6) implies that, H_2 number density is very low, $x_2 \approx 2Rn_{H0}(2Rn_{H0} + \zeta_{20}) \approx 4 \cdot 10^{-6}$ (we adopted a moderate estimate $n_{H0} = 1\ \mathrm{cm}^{-3}$). With the photon absorption taken into account and $\varphi_s = 0$, the medium presumably will be nonuniform. Indeed, the gas is mainly in atomic form close to bright stars. Far away from them, its considerable fraction may be in molecular phase.

At the first stage we calculated the gas structure including the H_2 production process and $\varphi_s = 0$, starting from the state with the aforementioned parameters. All calculations have been done for $\varpi = 5$ kpc, the angular rotation velocity of the spiral pattern $\Omega_p = 23\ \mathrm{km} \cdot \mathrm{s}^{-1} \cdot \mathrm{kpc}^{-1}$ (Marochnik *et al.*, 1972), and Schmidt's rotation curve. The profiles of different gas parameters after reaching a quasistationary state are given in Figure 2. As expected, atomic hydrogen prevails

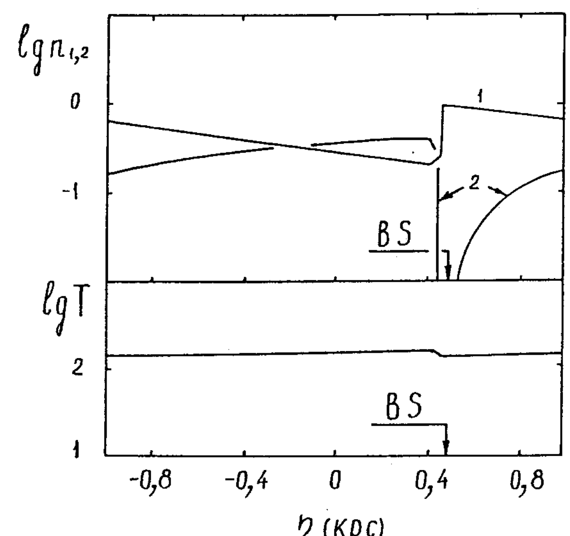

Figure 2 Gas parameters without the GDW ($\varphi_s = 0$); 1: $\lg n_1$; 2: $\lg n_2$. Bright stars location is marked by the arrow "BS".

near bright stars. Simultaneously, a significant fraction of the gas is in the molecular form. Calculations show that the ratio of the molecular hydrogen mass M_2 to the atomic mass M_1 is equal to $M_2/M_1 \approx 0.94$, that is nearly half of hydrogen mass is in molecular form.

At the second stage of calculations, the spiral field of the form

$$A = A_0[\exp(-\gamma\Omega t) - 1]$$

is included, where A_0 is the observed value of the GDW gravitational potential amplitude, γ is certain coefficient defining the GDW switching-on rate. According to Berman and Mishurov (1980), $A_0 \approx 248\,\text{km}^2 \cdot \text{s}^{-2}$ (this corresponds to the force amplitude of the spiral field of $F_* \approx 0, 1$) and $\gamma \approx 0, 2$ for a rather slow development of the GDW.

The gas flow in the ISM for a quasistationary state is illustrated by Figure 3. It

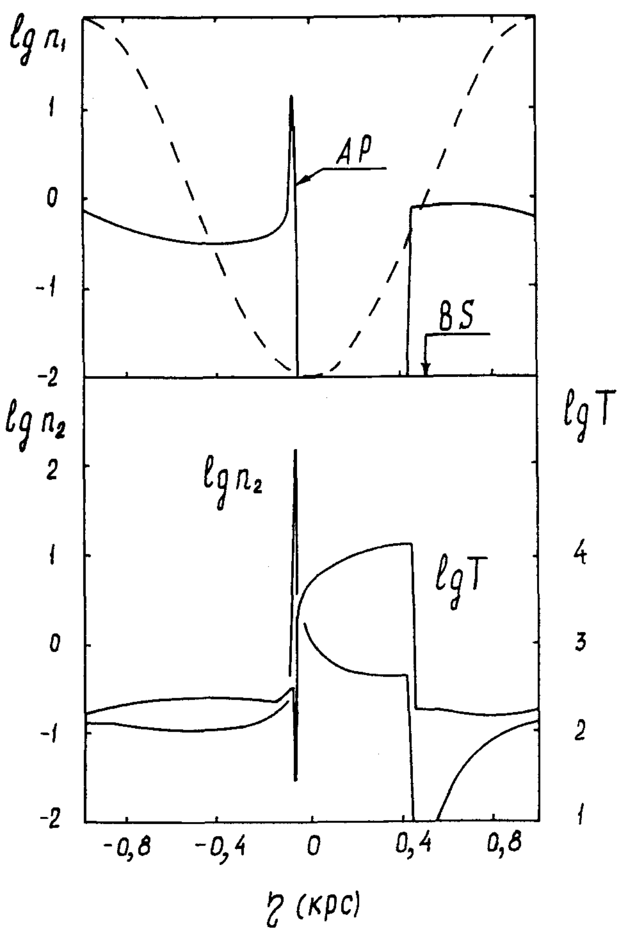

Figure 3 The same as in Figure 2, but with the spiral field included and after the gas flow has reached a quasistationary state. The atomic precursor is marked by the arrow "AP". Dashed line represents the dependence of $\varphi_s(\eta)$ in the arbitrary scale.

is clear that the fraction of molecular hydrogen is increased due to the accretion wave. This is easy to understand. On one hand, the H_2 formation rate is proportional to the gas density (strictly speaking, to the dust concentration, but the dust is carried away by the gas and concentrates where the gas density reaches a maximum). On the other hand, the molecule dissociation rate is lower in regions where the dust density and H_2 are higher. That is why accretion wave stimulates the transition of the gas into molecular form. Our results show that $M_2/M_1 \approx 1, 4$ in the presence of the GDW.

The chemical composition of a fluid element changes while it travels from one arm to another. When it approaches a bright stars region, its atomic hydrogen content practically equals 100%. And further, during a long period when the element is in the interarm region, atomic hydrogen still prevails in it. Violent H_2 formation occurs when the element finds itself in the AW where high gas density is reached. But even then H_2 molecule concentration exceeds the atomic gas concentration by an order of magnitude over the region of several hundred parsecs in size. The gas in the fluid element turns back into the atomic phase when it approaches again the neighborhood of bright stars.

4. DISCUSSION

Let us discuss some implications of our results. First of all, our calculations indicate that galactic density waves provide an efficient trigger mechanism for molecular hydrogen formation. Due to the AW, the H_2 mass fraction increases by a factor of approximately 1.5 in comparison to that without the GDW. Our simplified modes is only a rough approximation to the reality, and it hardly can be expected that all details of gas evolution and structure would find their explanation. But we believe that some aspects are reflected quite adequately.

Better possibilities for comparing the theory with observations arise when we turn to external galaxies. When looking at the galaxy from outside, the uncertainty in distances characteristic to the Milky Way is eliminated. Perhaps, the most suitable candidate for the purpose is M51. Recently, Vogel *et al.* (1988) and Tilanus *et al.* (1988) have investigated in detail, with the record resolution, the ISM structure in M51 using various tracers: CO, H_α, thermal and continuum emission. It turned out that a molecular arm is projected on dust lanes and synchrotron emission comes from here. Thermal spiral features coincide with the arms outlined by ionized hydrogen zones. Thus, the latter arm system (HI + HII) lies downstream of the former one (CO + dust + continuum) by 300–500 pc.

Such spatial structure of the ISM is readily explained in terms of our theory. Indeed, the coincidence of molecular and dust arms is not accidental: the dust is necessary for the molecule formation. In our calculations, the peaks of H_2 are achieved in the places where the dust concentration is maximum. But even in the region of width of 400 pc, the molecular hydrogen content exceeds the atomic hydrogen abundance by 1.5 orders of magnitude (Figure 3) and it is obvious that thermal radiation is suppressed here. This region must be visible mainly in the CO line.

Because of the restricted resolution achieved in the cited papers (~400 pc at the distance to M51), the observed in CO peak of H_2 is not so sharp as shown in

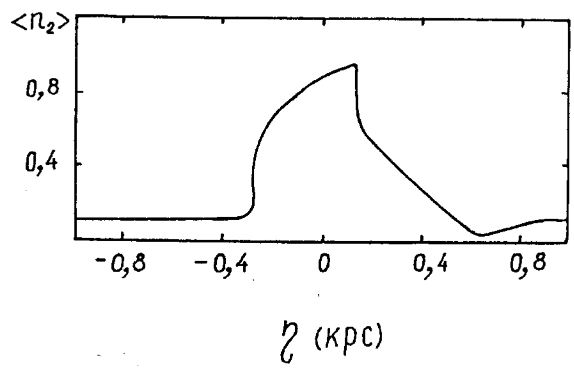

Figure 4 The profile of averaged H_2 density $\langle n_2 \rangle$ smoothed to the 400 pc resolution. The $\langle n_2 \rangle$ peak is displaced downstream of min φ_s position by about 100 pc.

Figure 3. Figure 4 shows the H_2 profile across the arm smoothed to the 400 pc resolution. After such smoothing, H_2 density and, consequently, the total gas and dust density reaches a maximum at the point slightly displaced (by ~100 pc downstream of min φ_s. This is what is observed in M51.

Furthermore, if the magnetic field is frozen into the gas, it is strongest in the region where the gas density is greatest, i.e., in the accretion wave. That is why the synchroton emission enhancement should be observed (as it does) in the molecular arm region.

According to our results atomic hydrogen, whose thermal emission is projected on the arms traced by H_α, results from dissociation of molecular hydrogen. Hence, it becomes clear why HI and HII arms coincide and the arm system is displaced downstream of the former one (CO + dust + continuum). Notice that the displacement between the arms (~400 pc) also agrees with observations. This confirms the idea of Cohen *et al.* (1980) that the gas spends some time in the atomic phase and some time in the molecular form. In other words, gas recirculation from the atomic form to the molecular and vice versa takes place.

Our model cannot explain all properties of the interstellar gas. For example, we obtain a rather high temperature for the region downstream of the H_2 peak in the AW. The reason is the fact that we do not allow for the molecular cooling (the gas is mainly in the molecular form in this region, see Figure 3). We hope that more realistic values of the temperature and structure of the gas can be obtained by including thermochemical important processes connected with H_2.

We consider important the prediction of a HI peak at the inner edge of a molecular arm (see Figure 3). We call it the "atomic precursor". It is sure to exist if molecular hydrogen really originates from atomic one due to reactions on dust grains. Indeed, for H_2 formation to be effective, a rather high, supercritical number density of HI is required. Some comments relevant to this phenomenon predicted by us can be found in Grabelsky *et al.* (1987) and Gosachinskij *et al.* (1988), who notice that molecular complexes are surrounded by HI envelopes. However, this observation refers to the Milky Way where distances cannot be determined unambiguously. Therefore, the detection of this phenomenon in external galaxies would provide a more direct confirmation. Unfortunately, the resolution achieved in the case of M51 is not high enough to detect the atomic precursor. The resolution of 4–5 times higher seems to be necessary for this purpose.

In this paper we have not considered some important problems, e.g. molecular cloud formation. We plan to discuss this and other problems in our subsequent papers.

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