

On temperature T_{01} for molecular hydrogen

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Abstract: Temperature T_{01} for hydrogen molecule for the transition between the level $J = 1$ (ortho- H_2) and the level $J = 0$ (para- H_2) has been introduced by Spitzer et al. [1]. The work of Spitzer et al. [1] has been reinvestigated and we find that the concept of the temperature T_{01} is not valid.

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Hydrogen molecule (H_2) comprising of two hydrogen atoms, is the lightest and most abundant molecule in the interstellar space. Nuclear spins of the atoms can have two combinations: $I=0$ (anti-parallel spins) and $I=1$ (parallel spins), and thus the molecule has two species, named para and ortho, respectively. In the ground electronic and ground vibrational states, the rotational levels with even J belong to the para-species whereas those with odd J belong to the ortho-species. Hence, there are two disjoint sets of rotational energy levels of H_2 molecule, one having levels with even J and the other having levels with odd J . The probability of any transition between ortho and para species of H_2 (*i.e.*, a transition between odd J and even J) is negligible. Spitzer et al. [1], however, envisaged that at the temperatures below 200 K, the ratio of N_1 (number of molecules cm^{-3} in the level $J = 1$) to N_0 (number of molecules cm^{-3} in the level $J = 0$) can be expressed by the usual Boltzmann formula

$$\frac{N_1}{N_0} = \frac{g_1}{g_0} e^{-E_{01}/kT_{01}}, \quad (1)$$

where g_1 and g_0 are the statistical weights of the levels, E_{01} the excitation energy of the level $J = 1$ above the level $J = 0$, and T_{01} the temperature corresponding to the number densities N_1 and N_0 .

Spitzer et al. [1] assumed that when hydrogen molecules were first formed on surface of grains, their population densities in the excited rotational levels followed the Boltzmann distribution formula. These populations subsequently cascaded down radiatively to the $J = 0$ and $J = 1$ levels, and therefore, they wrote

$$\frac{N_1}{N_0} = \frac{\sum_{\text{odd } J} g_J e^{-E_J/kT}}{\sum_{\text{even } J} g_J e^{-E_J/kT}}. \quad (2)$$

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Evidently, at low temperature, eq. (2) reduces to eq. (1). This expression (1) is being used extensively by the scientists [2], and by using the values of the population densities N_1 (in ortho-H₂) and N_0 (in para-H₂) in eq. (1), value of the temperature T_{01} is being derived.

Our first and the main objection about eq. (2) is that in the summations written on the right side of the equation, the energy in the exponential term must be the excitation energy, which is calculated relative to the energy of the lowest energy level of the system. For the case of para-H₂, this objection would not affect as the energy of the lowest level ($J = 0$) of the system is zero. However, it would affect for the ortho-H₂ as the energy of the lowest level ($J = 1$) of the system is not zero. When we deal with a system in which energy of the lowest level is non-zero, there is no way in the physical processes to remember the value of the energy of the lowest level. We always account for the energy of the levels relative to the energy of the lowest one [3].

Further, on the left side in eq. (2), there should be the ratio of the population densities of ortho-H₂ to para-H₂. Hence, in light of these points, the equation, corresponding to the eq. (2), should be written as:

$$\frac{N_{\text{ortho}}}{N_{\text{para}}} = \frac{\sum_{\text{odd } J} N_J}{\sum_{\text{even } J} N_J} = \frac{\sum_{\text{odd } J} g_J e^{-(E_J - E_1)/kT}}{\sum_{\text{even } J} g_J e^{-(E_J - E_0)/kT}} \quad (3)$$

In the low temperature regions, populations of the excited levels cascade down to the $J = 0$ (in para-H₂) and $J = 1$ (in ortho-H₂) levels, and thus, we have

$$\frac{N_{\text{ortho}}}{N_{\text{para}}} = \frac{N_1}{N_0} = \frac{g_1}{g_0} \quad (4)$$

which is physically a meaningful relation. Hence, it can be decided that the concept of the temperature T_{01} introduced by Spitzer et al. [1] is not valid.

After formation of ortho-H₂ and para-H₂ on the surface of grains, these two species behave like two independent molecules. The process of conversion of ortho-H₂ into para-H₂ is very similar to that of formation of one molecule from the other. The ratio of their number densities $N_{\text{ortho}}/N_{\text{para}}$ is similar to the ratio of number densities of two distinct molecules. The ratio $N_{\text{ortho}}/N_{\text{para}}$ or N_1/N_0 does not remember any thing about E_{01} (the excitation energy of the level $J = 1$ above the level $J = 0$) and thus, the question of computing T_{01} does not arise.

Some rotational energy levels of ortho-H₂ and para-H₂ in the ground electronic and ground vibrational states are given in Table 1. For these energy levels, the computed values of N_1/N_0 (eq. 2) and $N_{\text{ortho}}/N_{\text{para}}$ (eq. 3) for some kinetic temperatures are given in Table 2. Table 2 obviously shows that the concept of eq. (2) and therefore of eq. (1) is not valid.

Table 1: Rotational energy levels of H₂

ortho-H ₂		para-H ₂	
J	E(cm ⁻¹)	J	E(cm ⁻¹)
1	118.49	0	0.00
3	705.55	2	354.39
5	1740.22	4	1168.84
7	3187.36	6	2414.88
9	5002.03	8	4051.78
11	7135.94	10	6032.02
13	9545.72	12	8308.59
15	12203.25	14	10844.35

Table 2: Values of N_1/N_0 and $N_{\text{ortho}}/N_{\text{para}}$ for various temperatures

T (K)	N_1/N_0 [eq. (2)]	$N_{\text{ortho}}/N_{\text{para}}$ [eq. (3)]	T (K)	N_1/N_0 [eq. (2)]	$N_{\text{ortho}}/N_{\text{para}}$ [eq. (3)]
10	0.000	3.000	200	0.950	2.229
20	0.001	3.000	300	0.996	1.759
30	0.010	3.000	400	1.000	1.532
40	0.042	3.000	500	1.000	1.407
50	0.099	2.999	800	1.000	1.238
60	0.174	2.997	1000	1.000	1.186
80	0.353	2.975	1500	1.000	1.121
100	0.529	2.913	2000	1.001	1.090
120	0.677	2.806	3000	1.006	1.064
150	0.831	2.593	5000	1.025	1.060

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