Measurements of the Cosmic Microwave Background Temperature at high redshift by analysis of CO excitation

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Abstract. The linear relation between the temperature of the Cosmic Microwave Background and the cosmological redshift is a fundamental prediction of the standard hot Big Bang model. Measurements of the CMB temperature in the past can be done by means of observing radiative excitation of atomic and molecular species like C and CO. It can be detected in quasar spectra with \( z \sim 2 \). We study excitation of CO rotational levels both by the CMB radiation and collisions. Corrections of determination of the CMB temperature due to collisional excitation by the analysis of CO molecule rotation level populations are proposed.

1. Introduction
The Cosmic Microwave Background (CMB) is the thermal radiation left over from the early stages of the Universe. Its existence is a fundamental prediction of the hot Big Bang theory. In the standard cosmological model, the CMB undergo adiabatic expansion and the CMB black-body temperature has to be the linear function of redshift: \( T_{CMB}(z) = T_{CMB}^0 \cdot (1 + z) \), where \( T_{CMB}^0 = 2.7255 \pm 0.0006 \text{K} \) is the local CMB temperature [1]. However this relation can become nonlinear, e.g. \( T_{CMB}(z) = T_{CMB}^0 \cdot (1 + z)^{1-\beta} \) [2], if local position invariance is violated [3] or if the number of photons is not conserved. However, for the latter, it was shown [4] that is extremely difficult to fulfill “adiabatic” conditions, without producing the spectral distortions, which are constrained by FIRAS/COBEB at the level \( \delta I/I \sim 10^{-4} \) [5].

In that sense it is necessary to directly measure the evolution of \( T_{CMB} \). At low redshifts \( (z \lesssim 0.6) \) there is a method to determine \( T_{CMB} \) by using Sunyaev-Zeldovich effect [6], that is seen as CMB spectral distortions towards the galaxy clusters.

At higher redshifts \( (z \sim 2) \) \( T_{CMB} \) can be measured by analysis of the excitation of different atoms or molecules, which is measured using absorption lines in high redshift quasar spectra. To date populations of fine structure levels of C1 and rotational levels of CO are used.

In case of dominant excitation by the CMB radiation, the excitation temperature of this species is equal to the CMB temperature. The most stringent constraints on \( T_{CMB}(z) \) were obtained using CO rotational levels [3]. For the lowest vibrational level of the ground electronic state of CO the rotational transition energies between adjacent \( J-1 \) and \( J \) rotational levels are \( E_J = 5.54 \cdot J \text{K} \). Such energies are close to the CMB temperature, thus the rotational states of CO molecules are subject to the strong radiative excitation by CMB. However the presence
of CO molecules requires screening from UV radiation, since CO is easily photodissociated by UV photons. Therefore CO molecules are usually located in the center of a dense gas regions, which are refer to the translucent and dense molecular clouds. In such a dense medium the collisional excitation of CO molecules can be significant. In this work we examine the impact of the collisional excitation of CO on the CO excitation temperature that can be derived from the populations of the CO rotational levels.

1.1. \( T_{\text{CMB}} \) measurements based on CO molecules observations

Both absorption and emission lines of CO molecules are observed at high redshift. The study of CO absorption lines in quasar spectra allows one to separate a few components usually seen in CO profiles (which are shifted due to relative motions) and to measure accurately column densities of each rotational level for each component. Although CO molecule have a permanent dipole momentum and thereby have strong interaction with the radiation, the CO molecules were detected at high redshift in quasar spectra only recently in 2008-2011 [3, 8–10]. This is because of the complex CO chemistry: CO can be formed only in the medium that is well screened from the ambient UV radiation field, which destroys CO by photodestruction concerned with transitions in the resonance lines. The screening can be produced by the dust, \( \text{H}_2 \), and by the CO selfshielding that happens only in the deepest layer of interstellar clouds. At the same time such screening is preventing CO molecule from being detected since it absorb quasar spectrum as well. \( T_{\text{CMB}} \) measurements preformed by using analysis of CO absorption lines with high redshifts are summarized in [3]. These observations cover redshifts from \( z = 1.73 \) to \( z = 2.69 \) and were obtained neglecting the collisional excitation of CO molecules. Increase of the observation precision will require taking into account the collisional excitation.

2. Excitation of CO rotational levels by radiation and collisions

The radiative pumping of CO rotational levels via electronic transitions is negligible for the typical conditions of interstellar medium. Therefore the radiative excitation of CO rotational levels is dominated by CO pure rotational transitions. The main contribution of radiation at frequencies corresponding to these transitions (especially at high redshifts) is given by CMB radiation, which spectral energy distribution \( u(\nu) \) is well established to be blackbody. Therefore probabilities of rotational transitions between adjacent \((i + 1)^{\text{th}}\) and \(i^{\text{th}}\) states depend only on \( T_{\text{CMB}} \) and can be described as:

\[
W_{i,i+1}^{\text{CMB}} = B_{i,i+1}(\nu_{i,i+1}); \quad W_{i+1,i}^{\text{CMB}} = A_{i+1,i} + B_{i+1,i}(\nu_{i,i+1})
\]  

(1)

where \( \nu_{i,i+1} \), \( A_{i+1,i} \) and \( B_{i+1,i} \) are the frequency and Einstein coefficients of the \( i + 1 \rightarrow i \) transition, respectively. For our calculations we used these data taken from HITRAN\(^1\) database.

In case of a diffuse and translucent interstellar cloud it is sufficient to consider collisional excitation of rotational levels of CO molecules only by atomic hydrogen, molecular hydrogen and helium. To describe collisional transitions one needs to know its probabilities, number densities of all species that interact with CO molecules and the kinetic temperature of the gas, \( T_{\text{Kin}} \). Probabilities of collisional transitions are experimentally measured. For collisions of CO with atomic and molecular hydrogen we used data obtained by Yang et al. [11,12]. For collisions with helium we used data obtained by Cecchi-Pestellini et al. [13]. Since primordial helium to hydrogen ratio is well defined and can be taken equal to 0.083 [14], only three parameters determine collisional excitation of CO. It is convenient to take it as following: the total number density of particles, \( n \), the hydrogen molecular fraction, \( f = 2n(\text{H}_2)/(2n(\text{H}_2) + n(\text{H})) \) (which specifies molecular hydrogen abundance), and the kinetic temperature of the gas, \( T_{\text{Kin}} \). One can note that parahydrogen and orthohydrogen contribute differently in collisional excitation of CO

\(^1\) [http://hitran.iao.ru/](http://hitran.iao.ru/)
molecules and should be treated as two species. However in the considered self-shielded regions of H$_2$ medium their ratio is defined by $T_{\text{Kin}}$ and thereby the number of parameters remains the same.

The population of the CO molecule rotational levels can be expressed by number densities, $N_i$, of each CO level. In stationary condition one can write the detailed balance for $i$th rotational level.

$$\sum_{i \neq j} W_{ij} N_j - \sum_{j \neq i} W_{ji} N_i = 0,$$

where $W_{ij}$ is a probability of rotational transition from the state $i$ to the state $j$ that can be expressed as follows:

$$W_{ij}^{\text{tot}}(T_{\text{CMB}}, T_{\text{Kin}}, n, f) = \left\{ \begin{array}{ll}
\frac{f}{2} \left[ \alpha_{\text{para}}(T_{\text{Kin}}) W_{ij}^{H_{\text{2para}}}(T_{\text{Kin}}) + (1 - \alpha_{\text{para}}(T_{\text{Kin}})) W_{ij}^{H_{2\text{ortho}}}(T_{\text{Kin}}) \right] \\
+ (1 - f) W_{ij}^{H}(T_{\text{Kin}}) + 0.083 \cdot W_{ij}^{H_{\text{e}}}(T_{\text{Kin}}) \right\} \frac{n}{1.083 - f/2} + W_{ij}^{\text{CMB}}(T_{\text{CMB}}) \\
\end{array}\right.$$

where $\alpha_{\text{para}}$ is a fraction of parahydrogen. $W_{ij}^{H_{\text{2para}}}$, $W_{ij}^{H_{2\text{ortho}}}$, $W_{ij}^{H}$ and $W_{ij}^{H_{\text{e}}}$ are the probabilities of transitions from $i$ to $j$ rotational level of CO by collisions with para-H$_2$, ortho-H$_2$, H and He, respectively. A stationary solution of eq. 2, $N^{\text{CO}}$ (the vector describing the relative population of rotational levels of CO), is an eigenvector in the null space of the following matrix:

$$\tilde{W}_{ij} = W_{ji}^{\text{tot}} - \delta_{ij} \sum_k W_{ik}^{\text{tot}}$$

To summarize, $N^{\text{CO}}$ is defined by radiative and collisional transitions, which are determined by medium parameters $T_{\text{CMB}}$, $T_{\text{Kin}}$, $n$, and $f$.

### 3. Results

The figure shows the dependence of relative population of second and first excited rotational states compared to the population of the ground state of CO molecule on the total number density of gas. For this calculation we fixed $T_{\text{Kin}} = 100$ K, which is the typical kinetic temperature, measured in H$_2$-bearing clouds at high redshifts, and $T_{\text{CMB}} = 9.54$ K (that corresponds to the typical redshift of absorption systems, $z \approx 2.5$). We present the result of calculation in two limits: all hydrogen in the molecular phase, $f = 1$, (shown by red lines) and all hydrogen in the atomic phase, $f = 0$ (shown by blue lines). It can be seen that collisional excitation of CO by molecular hydrogen is more significant than excitation by atomic hydrogen in astrophysical conditions [15,16].

We have checked that our calculations satisfy the limiting cases: at low and high number density the relative population approaches the equilibrium distribution with the temperature equal to $T_{\text{CMB}}$ and $T_{\text{kin}}$ temperature, respectively:

$$N_{ij}^{eq}(T) = (2J + 1) \exp(-\frac{E_J}{kT})$$

Also we compare calculated relative populations of CO levels with the outputs from Radex [17] in case of collisions with molecular hydrogen only. In general, population distributions are consistent. However differences are growing with the level number. We measured average relative difference at the set of typical parameters: $T_{\text{CMB}} = 9.54$ K, $T_{\text{Kin}} = 100$ K, and $n = 200$ cm$^{-3}$. For the first three levels ($J=0,1,2$), the value is about $2 \cdot 10^{-4}$. For the first 6 levels, the value
Figure 1. Dependence of CO levels relative populations on the total particle concentration. Red and blue lines show cases of molecular and atomic hydrogen, respectively. Dashed lines correspond to the first excited states, and solid lines correspond to the second excited states. Limiting values with equilibrium CMB temperature and kinetic temperature represented by green and black lines.

is about $2 \cdot 10^{-3}$. And for 16 levels, average relative difference is about $10^{-2}$. This is probably due to different constants used in calculations.

It is worth mentioning that at high number densities $n \gtrsim 2000\, \text{cm}^{-3}$ inverse population of CO rotational levels is obtained, i.e. $N_1/N_0 > g_1/g_0 = 3$. The inverse population of the first rotational level occurs since the transition from the second to the first excited state at such number densities is mainly due to radiative transition, while all other transitions are dominated by collisional transitions. Thus the population of the first excited state of CO molecules is increased relative to the equilibrium state with the temperature equal to the kinetic gas temperature. Such behavior of the CO excitation temperature well agree with calculations performed by Varshalovich & Khersonskii in 1978 [18] for the local $T_{\text{CMB}}$.

The figure 2 shows the excitation diagram of CO rotational levels for the set of typical parameters: $T_{\text{CMB}} = 9.54\, \text{K}$, $T_{\text{Kin}} = 100\, \text{K}$, and $n = 200\, \text{cm}^{-3}$. Although, excitation temperatures differ for each transition, the determined excitation temperature describes rotational level populations relatively good. At higher levels the intensity of spontaneous emission drops below the intensity of collisional transitions. This leads to the change in the population distribution behavior starting from 6th excited rotational level.

At low number densities (up to few hundreds per cubic centimeter) our calculation demonstrates (see Fig. 1) that the excitation temperature differs little from the CMB temperature. It means that collisional excitation leads to the correction for measurement of $T_{\text{CMB}}$ from the observed excitation temperature of CO. It is convenient to formulate this correction for $T_{\text{CMB}}$ in an approximate way.

Figure 3 shows the dependence of estimated excitation temperature of CO molecules on the number density calculated at fixed $T_{\text{Kin}} = 100\, \text{K}$ and $T_{\text{CMB}} = 9.54\, \text{K}$. We have determined the excitation temperature of CO as averaged excitation temperature of the first two rotational
Figure 2. Excitation diagram of the first 9 rotational levels of CO for fixed $T_{\text{CMB}} = 9.54$ K, $T_{\text{Kin}} = 100$ K, and $n = 200$ cm$^{-3}$. Blue line corresponds to the determined excitation temperature and red line corresponds to the CMB temperature.

Figure 3. Dependence of the excitation temperature of CO molecules on total number density of the medium, for fixed $T_{\text{Kin}} = 100$ K and $T_{\text{CMB}} = 9.54$ K.

levels. To estimate the excitation temperature from modeled populations we have used unweighted $\chi^2$ criteria. As can be seen $T_{\text{Exc}}$ dependence on the particle number density for different molecular fractions of hydrogen is very close to linear one. Usually in observations
Figure 4. Dependence of the estimated correction for the CMB temperature on the kinetic gas temperature for different hydrogen molecular fractions. Figure presents approximation (lines) and calculated values (dots).

populations of the exited states of CO is obtained and $T_{\text{Exc}}$ is derived. Thus correction for $T_{\text{CMB}}$ taking into account collisional excitation of CO molecules can be expressed as linear function of the number density:

$$T_{\text{CMB}} = T_{\text{Exc}} - n \cdot \Theta(f, T_{\text{Kin}}, T_{\text{Exc}})$$

(6)

We found that in first order it depends only on the difference between the kinetic and the CMB temperatures. We proposed a fit function as following:

$$\Theta(f, T_{\text{Kin}}, T_{\text{Exc}}) = C_1(f)(1 - \exp(-C_2(f)(T_{\text{Kin}} - T_{\text{Exc}}))) + C_3(f)(1 + C_4(f)T_{\text{Exc}})(T_{\text{Kin}} - T_{\text{Exc}})$$

(7)

The approximation constants were obtained by comparison of the considered approximation with the calculated $T_{\text{Exc}}$ on the grid of $T_{\text{CMB}}$ and $T_{\text{Kin}}$ parameters: $T_{\text{CMB}}$ was varied from 7K to 13K with 1K step, $T_{\text{Kin}}$ was varied from 30K to 100K with 10K step, and $n$ from 0 cm$^{-3}$ to 500 cm$^{-3}$ with 50 cm$^{-3}$ step. The figure 4 shows the approximations for the excitation temperature. The approximation constants for different molecular fractions are presented in the table 1.

$$T_{\text{CMB}} = T_{\text{Exc}} - n \cdot \{C_1(f)(1 - \exp(-C_2(f)(T_{\text{Kin}} - T_{\text{Exc}}))) + C_3(f)(1 + C_4(f)T_{\text{Exc}})(T_{\text{Kin}} - T_{\text{Exc}})\}$$

(8)

Eq. (8) gives the estimated CMB temperature taking into account collisional excitation of CO molecules for the range of the total number densities.
Table 1. The approximation constants for $\Theta$ as a function of the molecular fraction $f$

| $f$ | $C_1$, $K \cdot cm^3$ | $C_2$, $K^{-1}$ | $C_3$, $cm^3$ | $C_4$, $K^{-1}$ | rms error | max error |
|-----|----------------|----------------|----------------|----------------|------------|-----------|
| 0   | $1.241 \cdot 10^{-3}$ | $1.784 \cdot 10^{-2}$ | $2.693 \cdot 10^{-5}$ | $2.633 \cdot 10^{-2}$ | $7.4 \cdot 10^{-3}$ | $2.9 \cdot 10^{-2}$ |
| 0.5 | $2.186 \cdot 10^{-3}$ | $3.195 \cdot 10^{-2}$ | $2.734 \cdot 10^{-5}$ | $3.363 \cdot 10^{-2}$ | $9.4 \cdot 10^{-3}$ | $3.4 \cdot 10^{-2}$ |
| 1   | $4.581 \cdot 10^{-3}$ | $3.542 \cdot 10^{-2}$ | $2.404 \cdot 10^{-5}$ | $5.499 \cdot 10^{-2}$ | $1.2 \cdot 10^{-2}$ | $4.8 \cdot 10^{-2}$ |

4. Conclusions

We have calculated the population distribution of the CO molecule rotational states taking into account radiative and collisional excitations. The impact of collisional excitation by $H$, $H_2$, $He$ on the level populations of CO molecules has been analyzed. We have confirmed that collisional excitation by atomic hydrogen is less significant than by molecular hydrogen in typical astrophysical conditions. Also it was shown that the appearance of an inverse population in CO molecules by a combination of collisional and radiative excitation is possible. Correction due to collisional excitation for determination of the Cosmic Microwave Background temperature at high redshifts by observations of populations of CO rotational levels has been calculated. We have derived approximation for this correction and its dependence on physical conditions in the interstellar medium (number density, kinetic temperature and molecular fraction).

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