DIATOMIC ANALYTIC MOLECULAR PARTITION FUNCTIONS FOR STELLAR ATMOSPHERES

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RESUMEN

Se formulan funciones de partición aproximadas y sus derivadas para moléculas diatómicas tomando en cuenta el número finito de niveles. Se desarrolla además un procedimiento para obtener expresiones analíticas compactas, sin parámetros libres, necesarias para la evaluación eficiente de algunos coeficientes termodinámicos de la función de partición para moléculas diatómicas de utilidad en el modelado de atmósferas estelares de baja temperatura.

ABSTRACT

Approximate partition functions and their derivatives for diatomic molecules are formulated taking into account the finite number of levels. A procedure is developed to derive compact analytic expressions, without free parameters, necessary for the efficient evaluation of some thermodynamic coefficients from the partition functions for diatomic molecules useful in modeling low temperature stellar atmospheres.

Key Words: equation of state — plasmas — stars: atmospheres

1. INTRODUCTION

To evaluate the partition function for the vibrational and rotational states of the diatomic molecules the maximum numbers of vibrational and rotational states in diatomic molecules in a partially ionized and dissociated perfect gas in thermodynamic equilibrium are very important for the numerical calculation of stellar atmospheres. The objective of this work is to develop fast and efficient analytic methods to calculate the partition functions from simple accurate expressions many times for a great number of diatomic molecules in the iterative processes necessary to evaluate the equation of state for cool stellar atmospheres and low density, low temperature plasmas. The partition function, called the sum over states or the grand sum (Zustandssumme) by Boltzmann, is the sum of the products of the statistical weights of the energy states of a molecule multiplied by the Boltzmann factors. In the calculation of the thermodynamic properties of a gaseous system, it is necessary to know the partition function for each chemical species in order to determine the populations in plasmas, planetary and stellar atmospheres, as well as some other thermodynamic coefficients through the use of the Helmholtz free energy, or using the Saha equation for ionization together with the molecular dissociation equation. In a perfect gas, the particles interact only through elastic collisions. The particles are immersed in a medium with a finite temperature and, therefore, governed by the internal energy of the gas; the fluctuations in energy broaden the lines (Cardona & Corona-Galindo 2012). When the partition function of diatomic molecules is evaluated, in most of the cases, the number of levels considered is taken as infinite and everything is evaluated with this assumption. The physical conditions of the thermodynamic system impose restrictions on the number of levels due to the broadening of the molecular lines (Cardona & Corona-Galindo 2012) in the molecules in the gaseous system composed of atoms, molecules and their ions. To derive analytic expressions for the partition functions we must transform the sums into integrals, supposing that the molecules have a great but finite number of states and, therefore, one can consider that the states form a continuum. In a great number of applications the partition functions are approximated by the statistical weights of the ground states

of the molecules, which produces poor results. The partition functions for diatomic molecules are relevant for the calculation of the equation of state in low temperature stellar atmospheres, where one wants to obtain the physical conditions from stellar atmospheres modeling. The diatomic molecules are very important in setting the atmospheric structure and the regions of instability for convection to occur inside the atmospheres. In what follows in § 2 we define the molecular states of diatomic molecules and the main thermodynamic variables. In § 3 we present the procedures for obtaining the vibrational and rotational partition functions for the heteronuclear and homonuclear diatomic molecules. The numerical results for the vibrational and rotational partition functions are given in § 4. Lastly, in § 5 some comments and conclusions about the procedure and results are given.

2. ENERGY STATES OF DIATOMIC MOLECULES

We consider a diatomic gas for which $k_{\mathrm{B}}T$ is small compared with the energy of dissociation E_{diss}; for different molecules this amounts to the condition: $T \ll E_{\mathrm{diss}}/k_{\mathrm{B}} \approx 10^4 - 10^5$ K, where k_{B} is the Boltzmann constant. At these temperatures the number of dissociated molecules in the gas would be quite insignificant. At the same time, in most cases, there would be practically no molecules in the excited electronic states as well, and the separation of any of these states from the ground state of the molecule is in general comparable to the dissociation energy itself. Accordingly, in what follows and in the evaluation of the partition function we take into account only the lowest electronic state of the molecule. Hence we consider only the vibrational and rotational states of the diatomic molecules in the developments that follow. As the number of states in diatomic molecules is not great (Cardona & Corona-Galindo 2012) the potential well is very close to the one of the harmonic oscillator and rigid rotator, a parabolic potential well. And, on the other hand, the third order terms in the potential are small and do not contribute to the sums of the partition functions. Therefore the third order terms do not influence the results whatsoever, because the sums are over states and these do not change for the finite number states for the given physical conditions, that is, the upper states are far away from the dissociation limit. Therefore we will use the harmonic approximation in our development.

2.1. *Vibrational states*

The vibrational energy states of a diatomic molecule derived from quantum mechanics (Herzberg 1950; Leighton 1959), for the intrinsic oscillator frequency ν_0, are given by the following expression

$$E_\upsilon = \left(\upsilon + \frac{1}{2}\right)\mathrm{h}\nu_0\,, \tag{1}$$

for $\upsilon = 0,\ 1,\ 2\ \ldots$, the vibrational quantum number, where h is the Planck constant. The oscillator intrinsic frequency is given by

$$\nu_0 \;=\; \frac{1}{2\pi}\sqrt{\frac{\mathrm{k}}{\mu}}\,, \tag{2}$$

with k the force constant of the oscillator and μ the reduced mass of the diatomic molecule.

2.2. *Rotational States*

The rotational energy states of a diatomic molecule derived from quantum mechanics for the moment of inertia I are expressed by

$$E_K \;=\; \frac{K(K+1)\mathrm{h}^2}{8\pi^2\mathrm{I}}\,, \tag{3}$$

for $K = 0,\ 1,\ 2\ \ldots$, the rotational quantum number.

2.3. *Thermodynamics of a gaseous system composed of diatomic molecules*

The main variables that describe a gaseous system in thermodynamic equilibrium are connected functionally by the equation of state. The equation of state of a system, composed by atoms, diatomic molecules and their ions, relates the temperature T, the pressure P and the total number density of particles N by the equation

$$P = N k_{\mathrm{B}} T, \tag{4}$$

where k_{B} is the Boltzmann constant mentioned before. With these variables, together with the partition function and taking into consideration the ionization and dissociation equations or the Helmholtz free energy, most of the thermodynamic coefficients can be derived.

3. PARTITION FUNCTION FOR DIATOMIC MOLECULES

The so called internal or molecular partition function for the diatomic molecules, for most of the applications, is composed of three independent partition functions that are the electronic, the vibrational, and rotational parts of the physical description of the molecules under the adiabatic approximation (Born & Oppenheimer 1927). The electronic transitions are of higher energy followed by the vibrational transitions of intermediate energy and the rotational transitions of lower energy. As was mentioned before, it is customary for the electronic transition to take into account only the lower energy states in the calculation of the general partition function; some results are given for the electronic partition function in Schadee (1964). There are situations where the adiabatic approximation breaks down (Bransden & Joachain 2003), but this is not in general the case for diatomic molecules (Brown & Carrington 2003) and for the physical conditions in stellar atmospheres and low density plasmas. Consequently, we will consider the vibrational and rotational partition functions separately and thus we can also compare directly each of them with the exact numerical evaluation of the partition functions. Using the results for the maximum number of rotational and vibrational states (Cardona & Corona-Galindo 2012) a procedure is developed to derive approximate compact analytic expressions, without any free parameters, forming a complete set of homogeneous equations necessary for the efficient evaluation of some thermodynamic coefficients of the partition functions for diatomic molecules useful for low temperature stellar atmospheres and low density laboratory plasmas.

3.0.1. *Vibrational partition function*

The vibrational partition function is defined by the following expression

$$Z_V = \sum_{v=0}^{\infty} e^{-\beta \Theta_V \left(v + \frac{1}{2} \right)}, \tag{5}$$

where $\beta = \frac{1}{k_{\mathrm{B}} T}$ and $\Theta_V = \hbar \omega_V$. This expression can be evaluated directly giving the following result

$$Z_V = \left(2 \sinh \left(\frac{\beta \Theta_V}{2} \right) \right)^{-1}. \tag{6}$$

But as the number of vibrational states is finite (Cardona & Corona-Galindo 2012) the evaluation of the sum can be carried out following the procedure presented below with the objective to obtain analytic equations. Dividing the sum into two parts, where the first sum contains few lower states and the second sum contains the rest of the states up to the maximum state, we have

$$Z_V = \sum_{v=0}^{v'} e^{-\beta \Theta_V \left(v + \frac{1}{2} \right)} + \sum_{v'}^{v^*} e^{-\beta \Theta_V \left(v + \frac{1}{2} \right)}, \tag{7}$$

where the sum to evaluate is defined by

$$Z = \sum_{v'}^{v^*} e^{-\beta \Theta_V \left(v + \frac{1}{2} \right)}, \tag{8}$$

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where dv/dN is given for different physical physical conditions in Cardona & Corona-Galindo (2012). In this case the exact derivative of the vibrational partition function with respect to N is the same as the one obtained above, and validates the procedure presented here.

For the derivative of the rotational partition function, equation (11) with respect to T one obtains

$$\frac{dZ_R}{dT} = \frac{g_n}{T\beta\Theta_R} \left[(1 + \beta\Theta_R)e^{-\beta\Theta_R} - (1 + \beta\Theta_R K^*(K^*+1))e^{-\beta\Theta_R K^*(K^*+1)} \right] , \tag{17}$$

and deriving with respect to N from equation (12) produces

$$\frac{dZ_R}{dN} = g_n K^*(K^*+1)e^{-\beta\Theta_R K^*(K^*+1)}\frac{dK^*}{dN} . \tag{18}$$

This is the exact derivative of the rotational partition function with respect to N. These equations for the partition function and its derivatives form a homogenous group of expressions for the heteronuclear diatomic molecules.

3.1. *Homonuclear diatomic molecules*

In the case of homonuclear diatomic molecules one has to take into account the degeneracy factor g_n due to the nuclear spins (Pathria 1972; Mohling 1982; Landau & Lifshitz 1980). The degeneracy factor is given by

$$g_n = (2S_1 + 1)(2S_2 + 1) , \tag{19}$$

for the possible orientations of the two nuclear spins (S_1 and S_2). For two nuclei, each with spin S, there are $S(2S + 1)$ antisymmetric spin states and $(S + 1)(2S + 1)$ symmetric ones. For diatomic molecules composed of identical Fermi nuclei ($S = 1/2, 3/2, ...$) one must therefore write the rotational partition function as

$$Z_R^{(F)} = S(2S + 1)Z_{\text{even}} + (S + 1)(2S + 1)Z_{\text{odd}} , \tag{20}$$

where

$$Z_{\text{even}} \equiv \sum_{K=0,2...}^{K^*} (2K + 1)e^{-\beta\Theta_R K(K+1)} , \tag{21}$$

and

$$Z_{\text{odd}} \equiv \sum_{K=1,3...}^{K^*} (2K + 1)e^{-\beta\Theta_R K(K+1)} . \tag{22}$$

For the case of diatomic molecules composed of identical Bose nuclei ($S = 0, 1, 2, ...$) one writes the rotational partition function as

$$Z_R^{(B)} = (S + 1)(2S + 1)Z_{\text{even}} + S(2S + 1)Z_{\text{odd}} . \tag{23}$$

Now, a change of variables in the equations (21) and (22) is performed. The even part is given by

$$Z_{\text{even}} = \sum_{K=0,1...}^{K^*} (4K + 1)e^{-\beta\Theta_R 2K(2K+1)} , \tag{24}$$

and transforming the sum into an integral the following result is obtained

$$Z_{\text{even}} = 1 + \frac{1}{2\beta\Theta_R} \left[e^{-2\beta\Theta_R} - e^{-\beta\Theta_R 2K^*(2K^*+1)} \right] . \tag{25}$$

The derivative with respect to temperature produces

$$\frac{dZ_{\text{even}}}{dT} = \frac{1}{2T\beta\Theta_R} \left[(1 + \beta\Theta_R)e^{-\beta\Theta_R} - [1 + \beta\Theta_R 2K^*(2K^* + 1)]e^{-\beta\Theta_R 2K^*(2K^*+1)} \right] , \tag{26}$$

and with respect to the total number density of particles gives

$$\frac{dZ_{\text{even}}}{dN} = (4K^* + 1)e^{-\beta\Theta_R 2K^*(2K^*+1)}\frac{dK^*}{dN}\,. \tag{27}$$

For the odd part the same procedure used above for the even part produces

$$Z_{\text{odd}} = \sum_{K=1,2...}^{K^*} (4K + 3)e^{-\beta\Theta_R(2K+1)(2K+2)}\,, \tag{28}$$

transforming the sum into an integral one obtains

$$Z_{\text{odd}} = \frac{1}{2\beta\Theta_R}\left[e^{-2\beta\Theta_R} - e^{-\beta\Theta_R(2K^*+1)(2K^*+2)}\right]\,, \tag{29}$$

the derivative with respect to temperature is

$$\frac{dZ_{\text{odd}}}{dT} = \frac{1}{2T\beta\Theta_R}\left[(1 + 6\beta\Theta_R)e^{-6\beta\Theta_R} - [1 + \beta\Theta_R(2K^* + 1)(2K^* + 2)]e^{-\beta\Theta_R(2K^*+1)(2K^*+2)}\right]\,, \tag{30}$$

and the derivative with respect to the total number density of particles is given by

$$\frac{dZ_{\text{odd}}}{dN} = (4K^* + 3)e^{-\beta\Theta_R(2K^*+1)(2K^*+2)}\frac{dK^*}{dN}\,. \tag{31}$$

where dK^*/dN is given for different approximations by Cardona & Corona-Galindo (2012). The expressions (26) and (29) should be used in equations (20) and (23), and the derivatives (26), (27), (30) and (31) in the derivatives of (20) and (23) with respect to temperature and to the total number density of particles. This completes the set of equations that represent the partition functions for the heteronuclear and homonuclear diatomic molecules and their derivatives for any application of the equation of state in low temperature stellar atmospheres and low density laboratory plasma spectroscopy, without the need of free parameters or polynomial adjustments. These results are very important for calculating stellar atmospheres models and this is the main reason for developing these analytic partition functions to model low temperature atmospheres. The equations of stellar atmospheres are nonlinear and nonlocal (Cardona, Crivellari, & Simonneau 2009) therefore one has to iterate these equations many times in order to obtain good results. For that reason we do not want to interpolate results of the partition functions developed in the literature mentioned in the articles. Our approximate analytic partition functions and their derivatives are also important for developing diagnostics of the physical conditions of plasmas of any type.

4. COMPARISONS AND NUMERICAL RESULTS

The expressions derived for the partition function are compared with some published results when possible. But in general one cannot compare the partition functions and the derivatives of the vibrational and rotational partition functions obtained above with other works because we do not have results for the separate vibrational and rotational partition functions and their derivatives. When there are results in the literature about the partition function they are obtained by truncating the sums to a prescribed value (Tatum 1966; Irwin 1981, 1988; Sauval & Tatum 1984; Rossi, Maciel, & Benavides-Soares 1985), or else the sums are evaluated with the upper limit set to infinity. Nevertheless, we can compare with the numerical evaluation of the exact vibrational and rotational partition functions, and with their derivatives with respect to temperature, using the definitions of the partition functions for the vibrational and rotational components with the upper limit set to the maximum number of states given by the physical conditions of the medium, and taking the molecular constants from different tables (Huber & Herzberg 1979; Cox 2000; Cohen, Lide, & Trigg 2003). Figure 1 shows the partition function evaluated from equation 10 and with the exact numerical calculation of the vibrational partition function for the heteronuclear molecule CH for the total number density of 10^{10} cm^{-3}. The results have relative errors of less than 0.1% for the range of the figure. Figure 2 shows the same results for a density of 10^{22} cm^{-3}, with the same relative error. In Figure 3 the rotational partition function is drawn for the
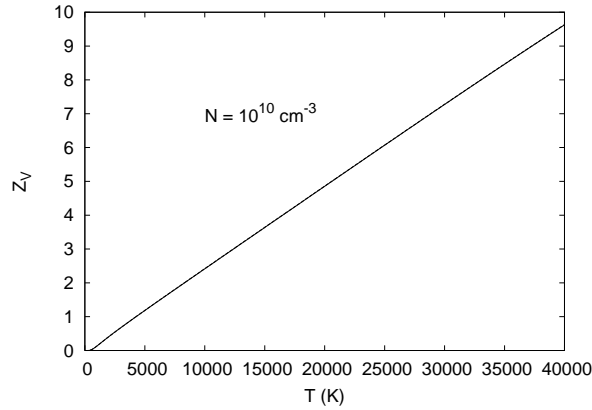
Fig. 1. Vibrational partition function for the diatomic molecule CH as a function of temperature for a total number density of particles of 10^{10} cm^{-3}. Exact partition function (solid line) and equation 10 (dots).

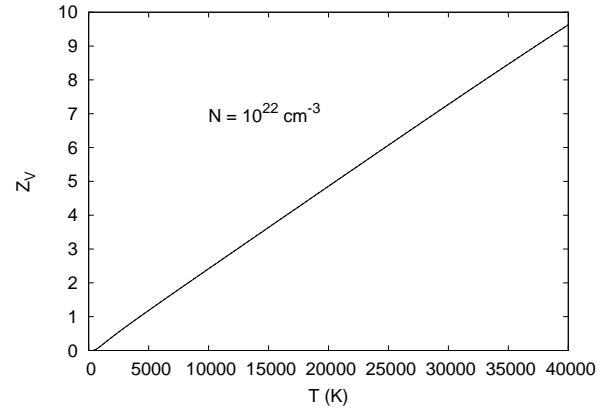Fig. 2. Vibrational partition function for the diatomic molecule CH as a function of temperature for a total number density of particles of 10^{22} cm^{-3}. Exact partition function (solid line) and equation 10 (dots).

Fig. 3. Rotational partition function for the diatomic molecule CH as a function of temperature for a total number density of particles of 10^{10} cm^{-3}. Exact partition function (solid line) and equation 14 (dots).
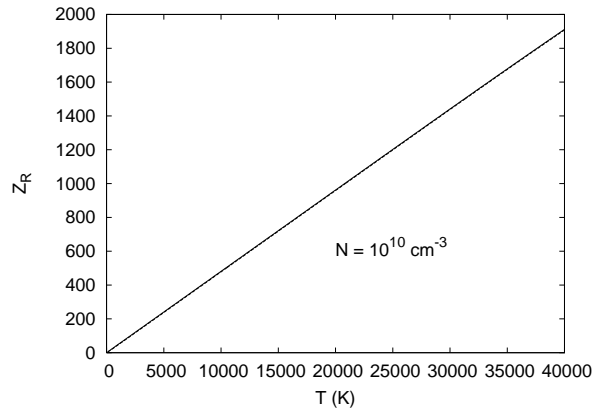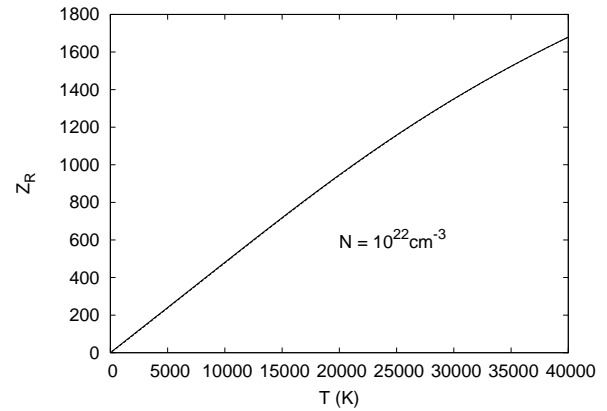

Fig. 4. Rotational partition function for the diatomic molecule CH as a function of temperature for a total number density of particles of 10^{22} cm^{-3}. Exact partition function (solid line) and equations 14 (dots).

exact partition function and equation 14 for a total density of 10^{10} cm^{-3}, with relative errors of less than 0.2% for the range of the figure. The degeneracy factor g_n divides the results, as it is customary. Figure 4 displays the differences in the high density and temperature regimes among the exact partition function and equation 14 for a total density of 10^{22} cm^{-3} with relative error of 0.5%. This shows the effect produced by few rotational states in these physical conditions, violating the assumptions made for the derivation of equation 14. In Figure 5 the derivative with respect to temperature for the vibrational partition function is drawn as a function of temperature and for total number density of 10^{10} cm^{-3}, for the exact result and for equation 15. Our result shows, close to the maximum, a relative error of the order of 0.4% comparing the exact result and the one calculated with equation 15, and less than 0.1% for the range of the figure with the same results for the total density of 10^{22} cm^{-3}, Figure 6. For the derivative of the rotational partition function the results have a relative error of less than 0.4% for the low temperature region, and of 0.05% for the rest, as shown in Figure 7 for a density of 10^{10} cm^{-3}. Figure 8 shows the derivative of the rotational partition function for a density of 10^{22} cm^{-3} with errors of 0.4% and 0.8% for the low and high temperature regions, respectively.

Fig. 5. Derivative of the vibrational partition function for the diatomic molecule CH with respect to temperature for a total number density of particles of 10^{10} cm^{-3}. Derivative of the exact partition function (solid line) and equation 15 (dots).
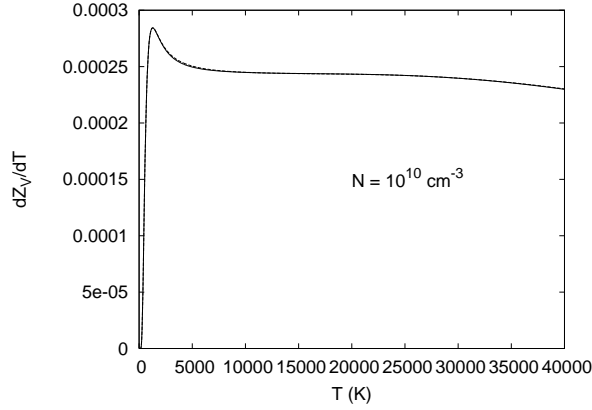
Fig. 6. Derivative of the vibrational partition function for the diatomic molecule CH with respect to temperature for a total number density of particles of 10^{22} cm^{-3}. Derivative of the exact partition function (solid line) and equation 15 (dots).

Fig. 7. Derivative of the rotational partition function for the diatomic molecule CH with respect to temperature for a total number density of particles of 10^{10} cm^{-3}. Derivative of the exact partition function (solid line) and equation 17 (dots).
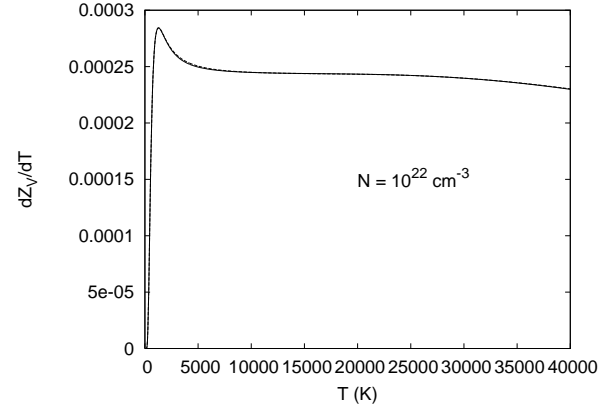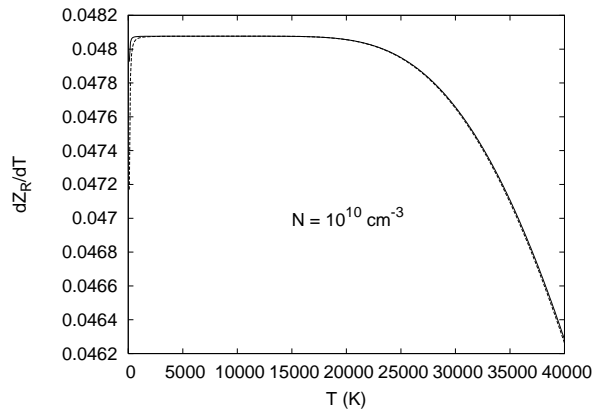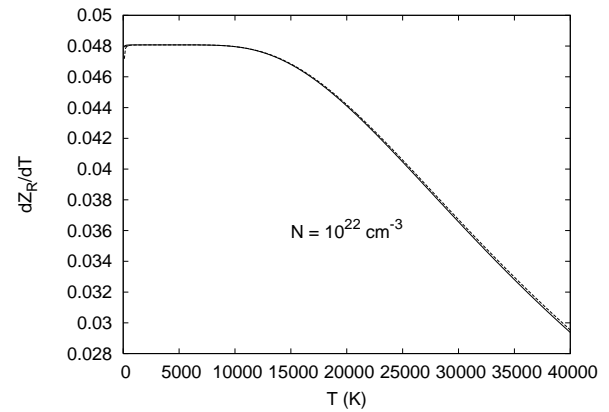
Fig. 8. Derivative of the rotational partition function for the diatomic molecule CH with respect to temperature for the total number density of particles of 10^{22} cm^{-3}. Derivative of the exact partition function (solid line) and equation 17 (dots).

The effect produced by few rotational states in these physical conditions, thus violating the assumptions made for the derivation of equation 17 is shown. The derivatives with respect to the number density of particles show a strange behavior below 10^3 K for both the vibrational and rotational partition functions, that appears to be due to resonances. This strange behavior of the partition functions is a numerical problem that can be corrected using the lowest terms of the power series of the exponentials. The CH molecule is important for cool stellar atmospheres because this molecule shows bands in solar type and low temperature stars (Kurucz, van Dishoeck, & Tarafdar 1987; Jorgensen et al. 1996). For the homonuclear molecule H$_2$ the rotational partition function is given in Figure 9 for a total number density of 10^{10} cm^{-3}, with relative error less than 0.5% in the low temperature region, and of 0.2% for the rest of the figure. Similar results are obtained for a total density of 10^{22} cm^{-3} as shown in Figure 10. In Figure 11 the derivative of the rotational partition function with respect to temperature is shown for a total number density of 10^{10} cm^{-3} and in Figure 12 for a total density of
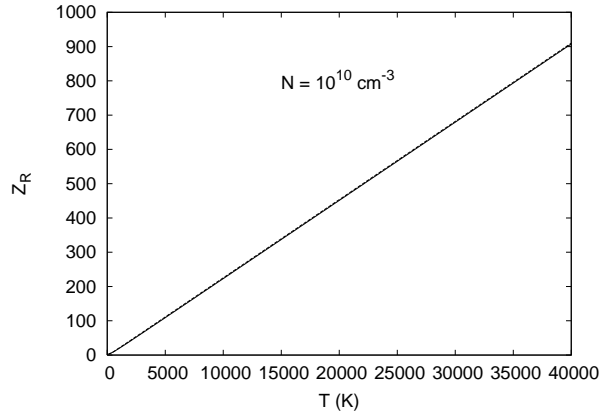
Fig. 9. Rotational partition function for the homonu-clear diatomic molecule H_2 with respect to temperature for a total number density of particles of 10^{10} cm^{-3}. Exact partition function (solid line) and equation 20 to-gether with equations 25 and 29 (dots).

Fig. 10. Rotational partition function for the homonu-clear diatomic molecule H_2 with respect to temperature for a total number density of particles of 10^{22} cm^{-3}. Exact partition function (solid line) and equation 20 to-gether with equations 25 and 29 (dots).
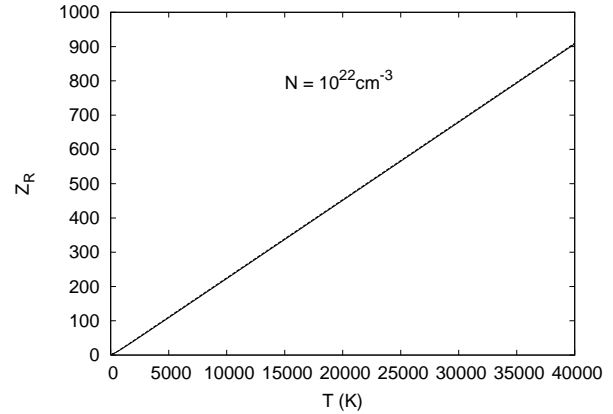

Fig. 11. Derivative of the rotational partition function for the homonuclear diatomic molecule H_2 with respect to temperature for a total number density of particles of 10^{10} cm^{-3}. Derivative of the exact partition function (solid line) and equation 20 together with equations 26 and 30 (dots).

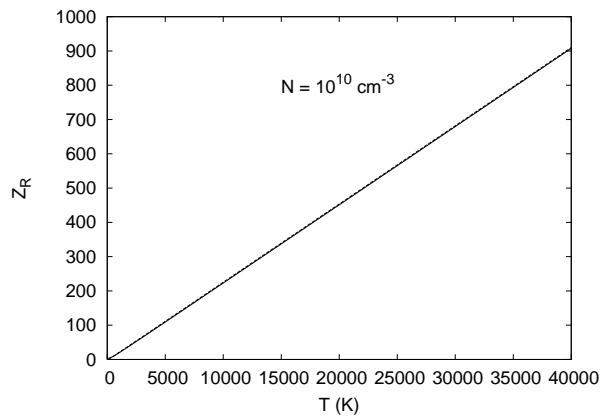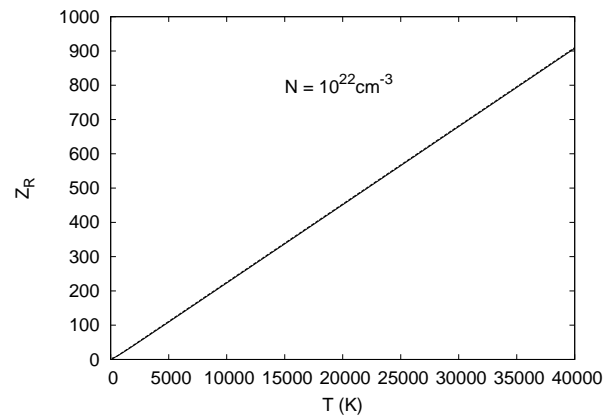Fig. 12. Derivative of the rotational partition function for the homonuclear diatomic molecule H_2 with respect to temperature for a total number density of particles of 10^{22} cm^{-3}. Derivative of the exact partition function (solid line) and equation 20 together with equations 26 and 30 (dots).

10^{22} cm^{-3}. The derivatives show values for the relative error of around 0.5% for the high temperature regime, but of less than 0.1% in the low temperature range of the values drawn, where again the problem of the number of levels appears. The vibrational partition function for H_2 shows the same behavior as the other heteronuclear molecules. For the vibrational partition function of homonuclear diatomic molecules is not necessary to consider the quantum statistics, as is the case for the rotational partition function of homonuclear diatomic molecules. Thus, the vibrational partition function is calculated in the same way as for any other heteronuclear diatomic molecule. Therefore for the hydrogen molecule we calculate the rotational partition function with the necessary quantum statistics for homonuclear molecules. The calculations for other molecules produce similar results as the ones presented above for the CH molecule, as is the case for the HCl molecule which is very important because many experimental results are available for it (Herzberg 1950; Leighton 1959; Eisberg & Resnick

1985). Therefore, these partition functions are very useful for approximating the vibrational and rotational partition functions for any type of diatomic molecules and their derivatives. They are simple to calculate in the evaluation of the equation of state for the construction of model atmospheres for low temperature stars. The figures displayed are essential, because they show the results with respect to the exact calculations of the partition functions and their derivatives for different total particle densities. These results are important for the calculation of the populations and other thermodynamic parameters in the modeling of stellar atmospheres and plasma diagnostics. To our knowledge, nowhere else can one find the derivatives of the partition functions with respect to the main thermodynamic variables; they are fundamental for the evaluation of the Helmholtz free energy and of the other thermodynamic coefficients using the Saha and dissociation equations, similarly to the case for atoms (Cardona, Simonneau, & Crivellari 2009). The figures display the results of the comparisons, giving good approximations for all the cases shown. In some of the figures one can appreciate very small differences between the exact and the calculated partition function and their derivatives, which should be taken into account. The absence of results published in the literature with respect to the exact partition functions prevented a comparison with our results. Therefore, the best comparison that one can make for the partition functions for diatomic molecules is with the exact calculations of the partition functions.

5. CONCLUSIONS AND COMMENTS

When one takes into account the interactions of the molecules with the medium in a gaseous system the number of vibrational and rotational energy states available becomes finite (Cardona & Corona-Galindo 2012). The partition functions derived using the results for the number of vibrational and rotational states in diatomic molecules are very general and simple, expressed in compact analytic equations that are functions of the maximum quantum numbers of the molecular states and of the main properties of the molecules only. That allows us for the first time to find the derivatives of the partition functions with respect to the total number density of particles in a natural way completing the set of equations for the calculation of the physical state of the material in stellar atmospheres of low temperature. The approximations made for the derivation of the analytic expressions are valid for molecules that have enough states given by the physical condition of the system under study. When the number of states is low one can calculate the exact partition function for these states. These partition functions form a homogenous group of analytic equations that can be used in any calculation of the equation of state for cool stellar atmospheres and low temperature plasmas. The partition functions and their derivatives with respect to temperature and total number density of particles are very helpful for calculating some thermodynamic coefficients for the radiative and convective transport of energy in stellar atmospheres.

We acknowledge the technical advice of María de los Ángeles López Castillo.

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