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A new way to measure the departure from thermodynamic equilibrium in stellar atmospheres *

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Abstract A new way to measure the departure from thermodynamic equilibrium is proposed based on the departure factor which evaluates the deviation from a Boltzmann level distribution, used by Short and Hauschildt (2005) and others. The way is based on an explicit relationship describing the departure factor as a function of line to continuum source, dynamic temperature and line photon frequency, under three assumptions that the scattering can be neglected, the background continuum can be treated as a Planck function, and finally the complete redistribution can be true. It has the advantage that the departure can be very conveniently evaluated from the spectral analysis with only the radiative transfer involved. Some physical insights are recovered for some extreme cases. Some example calculations of the departure are presented for the quiet Sun, faint solar flare and strong solar flare for the generally used solar chromospheric lines: Hα, Hβ, CaII H, K and triplet. It is revealed that in the case of solar flares, the departure is less than thermodynamic equilibrium along the larger depth range than in the quiet sun due to chromospheric condensation. It becomes hard to distinguish the departures for the different lines of the same atom or ion. It is expected that this investigation can be constructive for studying stellar atmospheres in cases where the three assumptions are close to reality.

Key words: line: formation — radiative transfer — stars: atmospheres

1 INTRODUCTION

The judgement of the thermodynamic state in a stellar atmosphere is very important in astrophysics, especially in stellar atmospheres where temperature is high and density is low. For instance, as initially pointed out by Mihalas (1978), a small departure from thermodynamic equilibrium (TE, and hereafter) will result in large errors in the abundance diagnostics in early-type stars. To specify the state of gas, the distribution of the particles (atoms, molecules, ions, free electrons, etc.) in different excitation and ionization states should be known. As is also well known, TE can be reached in the deepest layers of the stellar atmospheres, and roughly speaking, the higher in the atmosphere, the larger the deviation from TE. However, quantitative evaluation is needed for accurate computations. For instance, if the departure is comparably small, one can employ local thermodynamic equilibrium (LTE, and hereafter) as an approximation (Mihalas 1978).

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Whether the atmosphere is in TE or not can be judged by three conditions: 1) The Maxwell velocity distribution; 2) Boltzmann level distribution described by the Boltzmann excitation equation; and 3) the distribution among the occupation numbers of states of atoms or molecules of different ionization states being evaluated by the Saha ionization equation. However, it is worthwhile to note that Saha's distribution can be derived from the first two cases (Mihalas 1978).

The traditional evaluation of the departure from TE employs the factor ni/ni^*, where ni and ni^* are the occupation numbers of the bound level i in TE and non-TE respectively (Mihalas 1978). For instance, Przybilla and Butler (2004) used this factor when they studied the solar hydrogen spectrum in the non-LTE case. Though this definition is simple and closely connected to intuition, it suffers from the drawback that it is not available without the computations that include the statistical equilibrium equations (SEEs, hereafter), as generally written in the form (eqs. (5–87), Mihalas 1978)

$$\begin{aligned} &-\Sigma_{i''<i} n_{i''} (R_{i''i} + C_{i''i}) + n_i [\Sigma_{i''<i} (n_{i''}/n_i)^* (R_{ii''} + C_{i''i}) \\ &+\Sigma^k_{i'>i} (R_{ii'} + C_{ii'})] - \Sigma^k_{i'>i} n_{i'} (n_i/n_{i'})^* (R_{i'i} + C_{ii'}) = 0. \end{aligned} \tag{1}$$

Where R and C represent the radiation-induced and collision-induced transition rates respectively, and the subscripts indicate the energy levels. This action often makes the situation very intricate, and thus computationally expensive, as pointed out by Mihalas (1978). Furthermore, the computations are often atomic model dependent.

On one hand, because the radiation field and the states of atoms, ions or molecules are strongly coupled, if one deals with the issue of Non-LTE, the absolute occupation numbers are needed and a self-consistent simultaneous solution of both the radiative transfer and SEEs is required. On the other hand, the line parameters, like the line source function $S_{\rm l}$, the continuum source function $S_{\rm c}$, the line (radiation and collision) damping constant, the Doppler width, the line-of-sight velocity, etc. can be extracted only by inverting observational spectra as free parameters by using the radiative transfer equation, written as (eqs. (12–41), Mihalas 1978)

$$\mu dI_\nu/dz = -(\chi_{\rm c} + \chi_{\rm l}\phi_\nu) I_\nu + \chi_{\rm c} S_{\rm c} + \chi_{\rm l}\phi_\nu S_{\rm l}\,, \tag{2}$$

where I_ν represents the radiation field, $\chi_{\rm c}$ and $\chi_{\rm l}$ stand for the continuum and line center opacities, respectively, and ϕ_ν is the line profile. An issue may be raised about whether one can estimate the departure from TE without considering SEEs.

In the following section, one departure factor is given, which was used by Short and Hauschildt (2005) and its reciprocal by Anderson (1989) earlier. Its explicit relationship with the line to continuum source function ratio, the dynamical temperature, and the transition photon frequency is shown, which is in agreement with our previous work (Qu et al. 2006) under the assumptions: 1. the background continuum can be described by a Planck function; 2. the scattering can be ignored; and 3. the complete distribution can be realized. We recover the physical insights by viewing the relationship in some extreme cases and then follow by application of the calculations to the cases of the quiet Sun, as well as faint and strong flares for several frequently used lines.

2 RELATIONSHIPS BETWEEN DEPARTURE FACTOR, DYNAMIC TEMPERATURE, LINE TO CONTINUUM SOURCE FUNCTION RATIO AND LINE PHOTON FREQUENCY

First, one factor β is defined as

$$\beta \equiv \frac{S_{\rm l}}{S_{\rm c}}\,, \tag{3}$$

which depends on the number densities of the line emitters and absorbers, as well as the temperature. An important fact is that it can be extracted directly from the spectral analysis as one of the free parameters. The example can be found in our previous work (Qu et al. 2006), or both $S_{\rm l}$ and $S_{\rm c}$ can be extracted simultaneously (Lites et al. 1989). By identifying the Planck function as the continuum source function, and utilizing the expression of the line source function which contains the occupation numbers of the involved upper and lower levels (eqs. (4–14), Mihalas 1978),

$$Sl = \frac{2h\nu^3}{c^2}\Big[\frac{n_\mathrm{l}}{n_\mathrm{u}}\frac{g_\mathrm{u}}{g_\mathrm{l}} - 1\Big]^{-1}, \tag{4}$$

we found the relationship (eq. (6), Qu et al. 2006) between the departure factor γ from the Boltzmann level distribution (g_u and g_l are the statistical weights of the upper level and lower level respectively),

$$(n_\mathrm{u}/n_\mathrm{l})^* = g_\mathrm{u}/g_\mathrm{l} e^{\frac{-h\nu_\mathrm{ul}}{kT}}, \tag{5}$$

and β as

$$\begin{aligned}\gamma &\equiv \tfrac{n_\mathrm{l}}{n_\mathrm{u}}/(\tfrac{n_\mathrm{l}}{n_\mathrm{u}})^* \\ &= \tfrac{n_\mathrm{l}}{n_\mathrm{l}^*}/\tfrac{n_\mathrm{u}}{n_\mathrm{u}^*} \\ &= (\tfrac{e^{h\nu_\mathrm{ul}/kT}-1}{\beta} + 1)e^{-h\nu_\mathrm{ul}/kT} \\ &= \tfrac{1}{\beta} + (1 - \tfrac{1}{\beta})e^{-h\nu_\mathrm{ul}/kT} \\ &= 1/\beta(1 - e^{-h\nu_\mathrm{ul}/kT}) + e^{-h\nu_\mathrm{ul}/kT}.\end{aligned} \tag{6}$$

This factor is always positive, evidenced from the third or last equivalent equalities, and the derivation is independent of the radiative transfer. In the above equations, the asterisk $*$ indicates the quantities in TE, n_u and n_l are the occupation numbers of upper and lower levels of the concerned transition, and ν_ul is the frequency due to the transition, T is the kinetic temperature, h and k are the Planck and Boltzmann constants respectively.

Evidently, this factor depends on T, ν, as well as particle density on which β depends. It is worth noting that γ is only related to the relative occupation number distribution over the upper and lower levels of one radiative transition, and it varies from one pair of transition-related levels to another, which makes this factor different from the traditional one.

Because we employed Equation (4) of the line source function, the scattering is not included and the complete redistribution is employed. For the case where the scattering becomes important, the source function becomes much more complicated, as evidenced by equation (A25) of Vernazza et al. (1981).

It should be pointed out that the definition was not first given by us. In fact, a similar coefficient was introduced earlier by Vernazza et al. (1981), indicated by b_1 as (cf. their eq. (16))

$$b_\mathrm{l} = (n_\mathrm{l}/n_\mathrm{l}^*)/(n_k/n_k^*), \tag{7}$$

and k is referred to as the continuum. They calculated this factor by employing SEEs. Anderson (1989) gave one measure as

$$b_\mathrm{ul} = (n_\mathrm{u}/n_\mathrm{l})W_\mathrm{lu}, \tag{8}$$

where $W_\mathrm{lu} = (n_\mathrm{l}/n_\mathrm{u})^*$, which was called 'the Boltzmann-Saha ratio of state populations.' Note that $b_\mathrm{ul} = 1/\gamma$. It was regarded as the 'LTE departure coefficient for the upper state, relative to the lower state.' He calculated its value by the profile weighted mean intensity over the specific line transition $l \to u$, collisional de-excitation rates, Einstein rate coefficients (cf. eqs. (28–29), Anderson 1989). Though suitable for more general cases, this is a very different and complicated way to solve this issue. Short and Hauschildt (2005) recently followed Anderson's routine and also applied γ (say, their fig. 3) to the non-LTE situation by including SEEs. However, to the authors' knowledge, the explicit relationship, i.e., Equation (6), was first derived by us (Qu et al. 2006) in the simplified cases specified by the three assumptions outlined above.

At first glance, one can immediately see that when $\beta = 1$, i.e. $S_\mathrm{l} = S_\mathrm{c}$ is true in a stellar atmosphere, the departure disappears, and thus TE is recovered, as stated before (Qu et al. 2006). When β approaches unity, so does γ.

Let us first consider the situation when $\gamma < 1$, i.e., more particles from the lower state shift to the upper one relative to the TE case. This actually corresponds to the situation that $\beta > 1$ from the third equality of Equation (6), i.e., the line emission occurs. The departure becomes greater (less and less than 1) or the occupation number of the upper level increases as β increases. Therefore it can be concluded that if $\beta > 1$, the departure increases with β. In this case, the increase can also result from temperature enhancement, seen from the fourth equality. Similarly, if $\beta < 1$, corresponding to the absorption case, the departure increases as β or T decrease, evidenced by the last expression of Equation (6). Therefore, it can be summarized that the further the factor β is away from unity, the further the departure. Of course, the variation in β generally results from the variation in material density or/and temperature. This can help us to understand the reason why the LTE calculations cannot reproduce the observed line core profiles of Hα, Hβ, Hγ as well as $P\alpha$ formed in the solar atmosphere (Przybilla & Butler 2004). The physical contents hidden in Equation (6) can also be revealed from the following extreme cases.

First, when the temperature tends to infinity while the factor β is not so small, the departure factor tends to unity. This can be seen from the last three equalities of Equation (6). In fact, this case is equivalent to $h\nu_{\rm ul}/kT \ll 1$. Evidence can be found in the deepest layers (cf. fig. 3 of Przybilla & Butler 2004). However, this should be treated carefully. If the density is so low that the kinetic temperature makes no sense, or the thermal pool does not exist, the conclusion does not stand, like in the situation of the upper layers of the stellar corona. This is because the high temperature means high collision rate in dense enough matter. It occurs in the situation where the collision-induced transition rate is much higher than the radiation-induced one at this frequency, which is favorable for establishing TE. It should be noticed that as T increases, β also changes, but β's increase often cannot keep the cadence with that of T (say, cf., fig. 4 of Ding et al. 2002, as well as Ding et al. 1994). However, it should also be noticed that the conclusion stands when the assumptions are close to reality. From the upper chromospheric layers to the stellar corona, the scattering becomes more and more important and the complete redistribution cannot be valid for most of the lines, so the expression of $S_{\rm l}$ is invalid, and thus the Equation (6) cannot be applied and the above conclusion can no longer be true.

Second, if $h\nu_{\rm ul}/kT \gg 1$, from the fourth equality of Equation (6), one immediately obtains

$$\gamma = 1/\beta = S_{\rm c}/S_{\rm l}. \tag{9}$$

The factor β becomes the direct measure of the departure. This occurs when the radiation-induced transition rate dominates at frequency $\nu_{\rm ul}$, which can be found in the cool stars. This can help us to understand the departing behavior outlined by figure 3 of Przybilla & Butler (2004) for hydrogen Paschen lines in those curve segments where the temperature is low.

If $\beta \gg 1$, corresponding to the strong emission line case, say, for most of the non-scattering lines (especially some of the non-scattering ultraviolet ionized iron lines), from the third or last equalities, one obtains

$$\gamma = e^{-h\nu_{\rm ul}/kT}. \tag{10}$$

It is easily seen that the departure increases with the frequency exponentially, but decreases with T. In this case, the departure is independent of the particle density. From this result, along with the definition of γ and Boltzmann Equation (5), one can obtain, if $\beta \gg 1$,

$$\gamma = g_{\rm l} n_{\rm u}^* / g_{\rm u} n_{\rm l}^*, \tag{11}$$

which indicates that the departure can be evaluated by the TE calculation. Further, combining with the definition of γ, the ratio of the occupation numbers in this case is equal to their statistical weight ratio

$$n_{\rm u}/n_{\rm l} = g_{\rm u}/g_{\rm l}\,. \tag{12}$$

Therefore, it can be evaluated directly. This is equivalent to the case of TE when T becomes infinite.

However, if $\beta \ll 1$, which is representative of the strong absorption line case, from the fourth equality, it is obtained that

$$\gamma = 1/\beta(1 - e^{-h\nu_{\rm ul}/kT})\,. \tag{13}$$

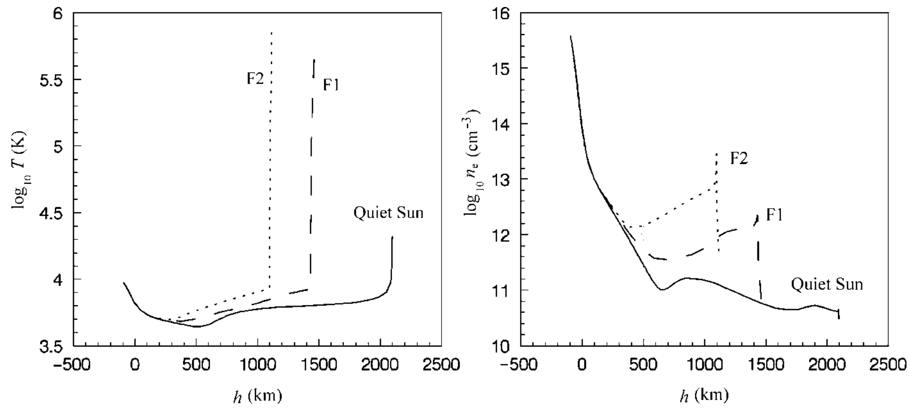

Fig. 1 The depth variations in temperature and electron density in cases of the Quiet Sun (VAL model), the faint solar flare (F1 model) and the strong solar flare (F2 model), respectively.

Evidently, it is still density dependent, for it relies on β. This is suitable for the strong absorption lines in the lower atmosphere. In this case, if $h\nu_{\rm ul}/kT \gg 1$, we again obtain the Equation (9). In the contrary case, i.e., if $h\nu_{\rm ul}/kT \ll 1$, one obtains

$$\gamma = 1/\beta \times h\nu_{\rm ul}/kT\,. \tag{14}$$

Now, let us keep the temperature and β constant to see the departing behaviors for lines with different frequencies, say, $P\alpha$, $P\beta$, $P\gamma$, Hα, Hβ, Hγ, etc. The fourth equality of Equation (6) shows that the increase of the frequency of the line photons, corresponding to the situation that the distance between the two levels becomes greater, will lead to the enhancementof the departure both in the emission ($\beta > 1$) and absorption ($\beta < 1$) cases. On the other hand, as pointed out by Vernazza et al. (1981), their $b_{\rm l}$'s 'generally approach unity with increasing l according to the enhanced collisional coupling between the higher levels and the continuum ...' This is also true for γ when both the upper and lower approach the continuum, because in this case, $\nu_{\rm ul} \to 0$.

3 SAMPLE CALCULATIONS OF THE DEPARTURE FACTORS FOR GENERALLY USED LINES IN SOLAR ATMOSPHERES

The significance of evaluating the departure factor lies in the application that it can tell us in which region one can apply LTE for specific lines. To illustrate this, we employ generally used solar lines for the quiet Sun, faint flares and strong flares, respectively. The model atmosphere of the quiet Sun was presented by Vernazza et al. (1981), hereafter referred to as the VAL model, and those of the faint and strong solar flares were given by Machado et al. (1980), hereafter referred to as the F1 and F2 models, respectively.

The left and right panels of Figure 1 outline depth variations in the temperature and electron density in the three cases. This figure was shown in Qu et al. (2002), but for convenience of discussion, it is plotted here again. One of the most outstanding differences between the quiet Sun and the flares lies in the fact that the density increases with temperature over depth domain where the layers are hit by high energetic particles from the arches. This results in very different departing behaviors between these two cases.

In order to show the departure in the solar atmosphere, one needs not only the model atmospheres, but also the calculations of the line parameters from the models by specific atom models. We adopt the calculations of $\mathrm{H}\alpha, \beta$ lines and CaII H, K as well as the triplet from Ding et al. (1994, 2002). From Figure 2, one can immediately see that from the quiet Sun through the faint flare to the strong flare, it

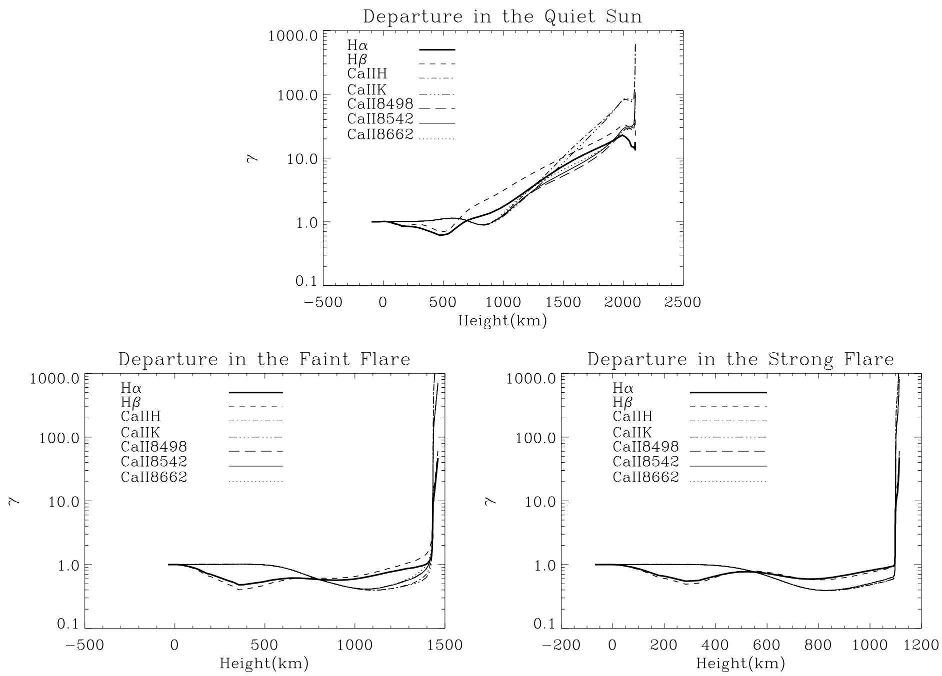

Fig. 2 The departure factor γ as a function of height in cases of the Quiet Sun (VAL model), the faint solar flare (F1 model) and the strong solar flare (F2 model) for the generally used solar chromospheric lines Hα,Hβ, CaIIH, CaIIK, CaII8498, CaII8542 and CaII8662 respectively.

becomes harder to distinguish the depth variation of the departure factor for different lines, while in the quiet Sun, one can distinguish the departure of one line from that of another line. A similar situation was met when we studied the line formation regions (Qu et al. 2002). In fact, in the two flare cases, the variation patterns can be divided into two groups according to the elements hydrogen and calcium which are involved. On the other hand, one fact which attracts us is that in the flare cases, over a much larger depth range than in the quiet Sun, the condition of the atmosphere more closely approaches TE. This is because in these layers (say, from $h = 500\,\mathrm{km}$ to $1000\,\mathrm{km}$), not only the temperature but also the number density increases with height (cf. Fig. 1) due to the chromospheric condensation (Gan et al. 1993a; Gan et al. 1993b; Gan et al. 1992), while in the quiet Sun, the overall density decreases. The increase in temperature and density helps the exchange of kinetic energies among the particles, and the collisional rate becomes high. This is more helpful for establishing the equilibrium. One can see that once the density drops abruptly while the temperature increases in all three cases, the departure becomes huge.

It should be noticed that we do not calculate the departure factors in sunspot penumbra or umbra. This is because, as pointed out by us (Qu et al. 2006), the occupation numbers of those atomic levels, whose Landé factors are non-zero, are changed exponentially with the magnetic field strength, and our evaluation is based on the departure from the Boltzmann distribution of the level populations. Only if the two levels from which the transition is deduced have a vanished Landé factor, can the departure be ascribed to that from TE.

4 DISCUSSION AND CONCLUSIONS

Under the assumption that the background continuum can be described by a Planck function, the scattering can be neglected and the complete redistribution can be applied. The relationship of the departure factor to the line to continuum source function ratio, line photon frequency and temperature are obtained. This provides a way to more clearly see its dependence on the physical parameters. However, it is time for us to outline the situations in which the three assumptions are true.

First, the way to treat the background continuum as a Planck function is valid when the thermal pool exists, or the density is not extremely low. Therefore, except in the outer corona, it is safe to do this. As pointed out, the scattering becomes important in the corona. In addition, the complete angular redistribution cannot exist in the corona where the geometry cannot be treated as symmetric, i.e., the anisotropy takes place. Thus, the evaluation of the departure based on the proposed way cannot be applied in the stellar corona. Finally, for the complete frequency redistribution, it is more suitable for the line core than in line wings. In fact the radiative transfer, described by Equations (2) and (4), can form a closed system that partially untangles the non-LTE issue of the two transition-related levels if one does not emphasize the absolute occupation numbers and the three assumptions are close to reality. This is because in some non-LTE cases, the parameters S_1, S_{c} and T can be extracted from the spectral analysis only by the radiative transfer. Once these parameters are obtained, the ratio $n_{\mathrm{u}}/n_{\mathrm{l}}$ can be derived from Equation (4), while the departure factor can be evaluated by Equation (6). This provides a way to estimate the error due to the LTE calculation. To further resolve the non-LTE issue when more energy levels of the atom are involved, one needs to observe more lines of the specific atom, and to do the same kind of analysis. The advantage of solving the non-LTE issue in this way is that it can be easily dealt with, and it is atomic model independent.

It should be stressed that, for domains absent of magnetic fields, it is safe to directly evaluate the departure from LTE by Equation (6). We found (Qu et al. 2006) that the magnetic field can exponentially increase the occupation number of the level having non-zero Landé factor, i.e., the magnetic field will cause the level population redistribution, thus source functions are changed accordingly. In this case, SEEs should be modified when those levels with non-zero Landé factors are included. Not only should this be done, but also the atomic model should be adopted very carefully. For instance, when the magnetic field is strong, those models omitting the levels with large Landé factors will cause significant errors. Therefore, not merely the radiation field causes the coupling between the radiative transfer and SEE, but also the magnetic field in this case. This makes the situation even more complicated. On the other hand, the situation described by Equation (6) indicates that the level distribution departs from the Boltzmann one without a magnetic field. In order to calculate the departure from TE, the influence of the magnetic field should be extracted. The same situation also exists if the departure is defined as n_i/n_i^*.

From the above analysis, it can be concluded that the advantages of the departure factor lies in the following aspects:

1. It is measurable directly from the spectral analysis by only utilizing the radiative transfer, for S_1 and S_{c} (and thus the kinetic temperature under the assumption) can be obtained as free parameters. The calculation of the departure is very simple according to Equation (6). However, the influence of the magnetic field should be extracted if one wants to get the real departure from TE when the magnetic field is present;
2. The calculation does not rely on atomic or molecular models, unlike those computations in which the model should be assumed for different purposes when the SEEs are included;
3. The physical insights can be more clearly obtained with Equation (6), and this can be applied to check the LTE calculation if the required conditions are satisfied.

Furthermore, as pointed out by Short & Hauschildt (2005), the significance of the factor also highlights the aspect that it measures the amount by which the population *ratio* of two levels within an ionization stage departs from the local Boltzmann ratio and is thus insensitive to non-LTE departures in the ionization balance.

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