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NUCLEAR β-DECAYS OF HIGHLY IONIZED HEAVY ATOMS IN STELLAR INTERIORS[†]

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Abstract: β-transition processes of heavy nuclei in stellar interiors are re-investigated. First, the relative abundances of ions in thermal equilibrium for given temperature, density and chemical composition are determined by solving the Saha ionization equation with the simultaneous inclusion of the continuum depression evaluated from a finite-temperature Thomas–Fermi model. Next, β-transitions in the equilibrated matter are studied. The numerical results for some selected examples demonstrate the need for such an involved treatment of β-decays (and particularly of bound-state β^- decays and orbital-electron captures) of certain nuclei of astrophysical importance.

1. Introduction

Nuclear β-transitions are known to play key roles at various stages of stellar evolution and in many nucleosynthesis processes. In such studies, one often encounters terrestrially unknown β-decay nuclear matrix elements between various levels of a supernova, or high-energy β^- decays of very neutron-rich nuclei [5–9]) presumably observed in many theoretical efforts to calculate the rates of, for instance, high-energy free-electron captures [1–4]) expected to play key roles in the collapsing core of a supernova, or high-energy β^- decays of very neutron rich nuclei [5–9]) presumably produced during the r-process nucleosynthesis. The results (or, the methods themselves) of these calculations are still in controversy mainly because of our lack of precise knowledge about β-strength functions [except those of light (e.g. sd shell) nuclei for which full shell-model calculations may be manageable [10])]. Such a knowledge for neutron-deficient heavy nuclei may also be requested in studies of the p-process [11]).

There are, on the other hand, those cases in which the relevant nuclear matrix elements are experimentally available or can be estimated rather accurately from (semi-)empirical systematics. Examples of this kind are found in the s-process which involves β-transitions mostly of low-lying states of nuclei near the line of β-stability. A drawback to this nice feature is caused by the fact that the ionization of the heavy atoms concerned is expected to be incomplete under plausible s-process

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conditions. This necessitates, at least in studies of orbital-electron captures, a detailed treatment of various ionic states in a plasma. Furthermore, whenever the β-transition energies are expected to be small, the energetics should be carefully handled with due consideration for the ionic energy differences which are then non-negligible and are sensitive to temperature and density. It is important to note that bound-state β^- decays [i.e. electron emissions into unoccupied bound-orbits [12,13])] could contribute significantly to low-energy β^- decays, and which might even overcome the usual continuum-state β^- decays by gaining comparatively large binding energies of the created electrons. [The global surveys of β-transition rates under s-process conditions [14]) are to be handled with some care, at least because of their neglect of bound-state β^- decay mechanisms.] Indeed, a few attempts have been made to study the bound-state β^- decays of certain heavy nuclei involved in the s-process [15,16]) or of ^{187}Re embedded in stellar interiors [17,18]). Their results, however, turn out to be highly questionable [19]) as their treatment of ionic states is oversimplified and the nuclear levels are selected in such a way that the most dominant β-transitions are often overlooked.

With this background, the present paper aims at a re-investigation of β-decays of highly-ionized heavy atoms in a plasma at temperatures T of 10^6–10^9 K and densities ρ of 10^{-4}–10^4 g/cm^3. The approximate nature of our treatment of the surrounding free electrons and ions as perturbers further restricts the T–ρ domain to which the following formalism can be applied: namely, in the high-ρ case, the low-T ranges are to be excluded. Still, the conditions considered here not only include the supposedly typical s-process conditions, but cover those which are realized during most of the stellar evolution phases. Aside from its application to the s-process branching problems [20,21]), and with the aid of stellar evolution models, the present formalism, therefore, also allows one to follow certain β-transmuting chronometric pairs (such as ^{187}Re–^{187}Os) from the time of star formation (at which time the elements are trapped from the interstellar medium) until practically the time of ejection [22]).

In sect. 2, the Saha equilibrium model is introduced to describe the system. It is coupled to a finite-temperature Thomas–Fermi model [23]) in order to simultaneously include the influence of the surrounding free electrons and ions in an approximate way, namely by means of the idea of "depression of the continuum". Various β-transition processes in the equilibrated matter are formulated in sect. 3. Some numerical results are discussed in sect. 4. Appendices supplement sect. 2 with some details.

2. Equilibrium model

2.1. SAHA IONIZATION EQUATION

Under the assumption of local thermodynamical equilibrium, the population of differently ionized states of a non-relativistic, non-degenerate element i (specified

by its nuclear charge and mass numbers) is obtained from the Saha ionization equation [24])

$$n_{ij+1}/n_{ij} = (b_{ij+1}/b_{ij})(M_{ij+1}/M_{ij})^{3/2} \exp[-\chi_{ij}/(\kappa T) - \eta], \tag{1}$$

where n_{ij} is the number density of element i in its j-times ionized state, b_{ij} the atomic partition function, M_{ij} the mass, χ_{ij} the ionization potential, κ the Boltzmann constant and T the temperature, while the electron degeneracy parameter η (i.e. the chemical potential without the rest mass $m_e c^2$ divided by κT) is related to the free electron number density n_e by

$$n_e = F(\eta, \beta)/(\pi^2 \lambda\!\!\!^{-3}), \tag{2}$$

where $\lambda\!\!\!^{-} = \hbar/m_e c$, $\beta = m_e c^2/\kappa T$ and the relativistic Fermi–Dirac integral

$$F(\eta, \beta) = \int_1^\infty W(W^2-1)^{1/2} f_{FD}(\eta, \beta)\, dW, \tag{3}$$

with

$$f_{FD}(\eta, \beta) = [1 + \exp(\beta(W-1) - \eta)]^{-1}. \tag{4}$$

The number density of positrons in an $e^- e^+ \rightleftharpoons 2\gamma$ equilibrium is obtained from eq. (2) with η replaced by $-\eta - 2\beta$. In the temperature and density ranges considered in the present paper, these positrons play no significant roles except in the marginal cases near the highest-temperature and lowest-density boundary. Therefore, and since the alterations necessary for its inclusion are quite straightforward, the positron abundance is neglected in the following formalism.

The total mass density ρ of a mixture of different elements with mass fractions x_i ought to satisfy the mass relationship

$$\rho x_i = \sum_j M_{ij} n_{ij}, \tag{5}$$

where $\sum_i x_i \simeq 1$ and the summation over j runs from zero to the respective atomic number Z_i. Combined with the charge neutrality, this leads to

$$\rho \sum_i x_i \left(\sum_j j n_{ij} \Big/ \sum_j M_{ij} n_{ij} \right) = n_e. \tag{6}$$

The abundances n_{ij} can now be obtained by iteratively solving eqs. (1)–(6) for a given set of T, ρ and x_i, provided that all of the b_{ij}, χ_{ij} and M_{ij} are known. It is clear that the replacements of M_{ij} by the neutral atomic mass M_{i0} and of $\sum_i x_i$ by unity in the above equations can be done without significant loss of accuracy.

2.2. ATOMIC DATA

The potential distribution in and near an ion is influenced not only by its own bound electrons, but also by the surrounding free electrons and neighboring ions.

The net effect of the electrostatic interactions of these "perturbers" on the internal states of an ion may be described as a depression of the continuum [24]: namely, the effective ionization potential χ_{ij} is expected to be smaller than the laboratory value I_{ij} by a certain amount Δ_{ij}, so that

$$\chi_{ij} = I_{ij} - \Delta_{ij} . \tag{7}$$

Since the experimental data are scarce for highly ionized heavy elements, the uncorrected ionization potentials I_{ij} are calculated from the relativistic self-consistent method of Liberman *et al.* [25].

The method of calculating the perturbation Δ_{ij} has been a subject of controversy [see e.g. ref. [24]]. Closely followed in the present work is the finite-temperature Thomas–Fermi model of Stewart and Pyatt [23] detailed in appendix A. As a result, Δ_{ij} in eq. (7) is replaced by Δ_j which is defined by eq. (A.13), and which depends only on the net ionic charge j once T, ρ and the composition are specified.

The atomic partition functions b_{ij} are defined by

$$b_{ij} = \sum_k b_{ijk} \exp(-e^*_{ijk}/\kappa T) , \tag{8}$$

where b_{ijk} and e^*_{ijk} are respectively the statistical weight and the excitation energy of the kth atomic level of the j-times ionized element i. As discussed in appendix A, the influence of the perturbing potential created by the free electrons and neighboring ions upon the single-particle energies is almost independent of electron orbits provided the density is not too high. Therefore, e^*_{ijk} may be regarded as laboratory energies. As for the summation in eq. (8), the conventional cut-off method is applied for simplicity: namely, the contributions from those levels whose excitation energies exceed the corrected ionization potential χ_{ij} are all excluded. For most of the heavy ions, the existing experimental data are hardly sufficient for calculating b_{ij}. Theoretical values can be derived from the single-particle eigen-energies [25] for the ground-state configuration by particle–hole excitations. The results obtained in such a way are very close to those derived self-consistently for each configuration. If that procedure still consumes too much computational time, as may be the case for heavy ions, a schematic hydrogen-like model with effective charges is adopted (see appendix B).

The above prescription seems to yield the atomic data within the accuracy requested in our present β-decay study, although a more sophisticated and more consistent approach with due consideration for the scattering states [26] shall definitely be called for in the future.

3. β-transition rates in stellar interiors

Restricting T and ρ in the ranges 10^6–10^9 K and 10^{-4}–10^4 g/cm^3, respectively, we discuss the following β-transition processes on heavy nuclei in the equilibrated

matter:

$$(Z, N, j; Kk)_{\mathrm{I}} \to (Z+1, N-1, j+1; K'k')_{\mathrm{F}} + \mathrm{e}^- + \bar{\nu}_{\mathrm{e}}$$
$$\text{continuum-state } \beta^- \text{ decay}, \tag{9a}$$

$$\to (Z+1, N-1, j; K'k')_{\mathrm{F}} + \bar{\nu}_{\mathrm{e}}$$
$$\text{bound-state } \beta^- \text{ decay}, \tag{9b}$$

$$\to (Z-1, N+1, j; K'k')_{\mathrm{F}} + \nu_{\mathrm{e}}$$
$$\text{orbital } \mathrm{e}^- \text{ capture}, \tag{9c}$$

$$\to (Z-1, N+1, j-1; K'k')_{\mathrm{F}} + \mathrm{e}^+ + \nu_{\mathrm{e}}$$
$$\text{continuum-state } \beta^+ \text{ decay}, \tag{9d}$$

and

$$(Z, N, j; Kk)_{\mathrm{I}} + \mathrm{e}^- \to (Z-1, N+1, j-1; K'k')_{\mathrm{F}} + \nu_{\mathrm{e}}$$
$$\text{free } \mathrm{e}^- \text{ capture}. \tag{9e}$$

Here, $(Z, N, j; Kk)$ stands for the initial state I or the final state F (before any secondary processes) specified by the proton number Z, neutron number N, and degree of ionization j (i.e. the number of bound electrons is equal to $Z-j$), while the variables K and k represent nuclear and atomic states, respectively. Under the considered stellar conditions, the (anti-)neutrinos (assumed to be massless) can escape freely without being trapped.

3.1. ENERGETICS

The Q-values of reactions (9a–e) in the case of *no* continuum depression are respectively given by

$$Q_0 = \begin{cases} q_0, & \text{(10a–c)} \\ q_0 - 2m_{\mathrm{e}}c^2, & \text{(10d)} \\ q_0 + K_{\mathrm{e}}, & \text{(10e)} \end{cases}$$

with

$$q_0 = [M_{\mathrm{I}0} - M_{\mathrm{F}0}]c^2 + [E^*_{\mathrm{I}K} - E^*_{\mathrm{F}K'}] + [B_{\mathrm{I}0} - B_{\mathrm{F}0}]$$
$$- [B_{\mathrm{I}j_{\mathrm{I}}} - B_{\mathrm{F}j_{\mathrm{F}}}] + [e^*_{\mathrm{I}j_{\mathrm{I}}k} - e^*_{\mathrm{F}j_{\mathrm{F}}k'}], \tag{11}$$

where M_{i0} $(i = \mathrm{I}, \mathrm{F})$ are the ground-state masses of the respective neutral atoms, E^*_{iK} the nuclear excitation energies, B_{ij} the total binding energies of bound electrons in the j-times ionized atomic ground-states, e^*_{ijk} the ionic excitation energies as in eq. (8), and K_{e} is kinetic energy of a free electron to be captured. The imperfect overlap of initial and final atomic states, which is caused by a sudden change of the nuclear charge by one unit, changes the Q-values by no more than 0.14 keV even for $Z = 92$ [ref. [27])]. Such a precision is beyond the one requested in the

present study of stellar β-transitions. Therefore, this non-adiabaticity effect on the energetics is simply ignored.

According to the result in subsect. 2.2, the corresponding Q-values *with* the continuum depression effect included as a perturbation can be approximated by

$$Q \simeq Q_0 + \sum_{j_I}^{Z_I-1} \Delta_j - \sum_{j_F}^{Z_F-1} \Delta_j , \tag{12}$$

in terms of Δ_j defined by eq. (A.13). Since Δ_j is positive and is greater for larger j, the continuum depression leads to a reduction of Q-values for the $Z \to Z+1$ transition (9a–b) and an increase for the $Z \to Z-1$ transition (9c–e). If these energy shifts become comparable to the unperturbed value Q_0, the approximation (12) fails because of our crude way of evaluating Δ_j.

3.2. TRANSITION RATES

3.2.1. Relation to terrestrial rates. In what follows, we explicitly deal with allowed and first-forbidden transitions which play decisive roles in determining the total β-decay rates of the vast majority of nuclei.

It is generally accurate enough to retain only the contributions from the possible lowest lepton partial waves [28]) [except eventually for such a case as RaE; see ref. [29])]. Classifying each β-transition as either allowed (a), non-unique first-forbidden (nu) or unique first-forbidden (u), we may then write the transition rates of reactions (9a–e) in the following form

$$\lambda_{\mathrm{IF}}^{(m)} = \begin{cases} [(\ln 2)/f_0 t] f^*_{\mathrm{IF}(m)} & \text{for } m = \mathrm{a}, \mathrm{nu} \\ [(\ln 2)/f_1 t] f^*_{\mathrm{IF}(m)} & \text{for } m = \mathrm{u}, \end{cases} \tag{13}$$

where use is made of the ft values of the corresponding "terrestrial" transitions [t being the partial half-life, and $f_0 \equiv f^{(\mathrm{a})} = f^{(\mathrm{nu})}$ or $f_1 \equiv f^{(\mathrm{u})}$ the usual f-functions [30])], while the function $f^*_{\mathrm{IF}(m)}$ expresses the respective lepton phase volume in stellar circumstances (subsect. 3.2.2).

If the relevant ft value is experimentally unknown or unattainable, as is often the case in astrophysical problems, the value from systematics (or, more precisely, that obtained from the systematics of reduced nuclear matrix elements) may be used. For allowed or unique first-forbidden transitions, the ft values of the inverse reactions can also be utilized if they are experimentally known or can be reliably estimated from systematics. In the case of non-unique first-forbidden transitions, this procedure has to be used with some caution since the cross terms of the nuclear matrix elements change signs for $Z \to Z+1$ and $Z \to Z-1$ transitions [28]). Those sign changes, however, mostly cancel out once the CVC [31]) and approximate relationships [32]) between the matrix elements are adopted. This implies that, even for non-unique transitions, one can utilize the ft values of the inverse transitions

with some confidence without knowing the hard-to-evaluate individual matrix elements.

3.2.2. Lepton phase volume in stellar condition. Here, the lepton phase volume functions $f^*_{\mathrm{IF}(m)}$ in eq. (13) are given for reactions (9a–e) in stellar conditions.

In the case of continuum-state $\beta^{\mp}$ decays,

$$f^*_{\mathrm{IF}(m)}(\mathrm{c.d.}) = \int_1^{W_{\max}} (W^2-1)^{1/2} W q^2 F_0 S_{(m)} f_{\mathrm{d}}\, \mathrm{d}W, \tag{14a,d}$$

where $W_{\max} = Q/m_{\mathrm{e}}c^2 + 1$ [eq. (12)], $q = W_{\max} - W$, F_0 is the so-called Fermi function [33]), the function f_{d} taking care of the Pauli principle is equal to $1 - f_{\mathrm{FD}}(\eta, \beta) = f_{\mathrm{FD}}(-\eta, -\beta)$ for β^- decays and to $1 - f_{\mathrm{FD}}(-\eta - 2\beta, \beta) = f_{\mathrm{FD}}(\eta + 2\beta, -\beta)$ [$\simeq 1$ in absence of appreciable positron abundance] for β^+ decays [see eq. (4)], and finally the spectral shape factors $S_{(m)}$ are given as

$$S_{(m)} = \begin{cases} L_0 & \text{for } m = \mathrm{a},\ \mathrm{nu} \\ q^2 L_0 + 9 L_1 & \text{for } m = \mathrm{u}, \end{cases} \tag{15}$$

where L_0 and L_1 are certain combinations [33,34]) of electron (or positron) radial wave functions evaluated at an appropriately chosen nuclear radius R.

Similarly, for continuum-state (free) e^- captures, one gets

$$f^*_{\mathrm{IF}(m)}(\mathrm{c.c.}) = \int_{W_{\min}}^{\infty} (W^2-1)^{1/2} W (Q/m_{\mathrm{e}}c^2)^2 F_0 S_{(m)} f_{\mathrm{c}}\, \mathrm{d}W, \tag{14e}$$

where $W_{\min} = 1$ if the Q-value is positive for zero e^- kinetic energy [i.e. $K_{\mathrm{e}} = 0$ in eqs. (12) and (10)], and $W_{\min} = 1 + |Q(K_{\mathrm{e}} = 0)/m_{\mathrm{e}}c^2|$ otherwise, while $f_{\mathrm{c}} = f_{\mathrm{FD}}(\eta, \beta)$.

For the bound-state β^- decay and bound-state (orbital) e^- capture processes,

$$f^*_{\mathrm{IF}(m)}(\mathrm{b.d./b.c.}) = \sum_x \sigma_x (\pi/2)[g_x \text{ or } f_x]^2 q^2 S_{(m)x}, \tag{14b,c}$$

where σ_x describes the vacancy (for bound-state β^- decays) or occupancy (for orbital e^- captures) of the electron orbit x and lies between zero and unity, $[g_x$ or $f_x]$ is understood to be the larger component of the electron radial wave functions evaluated at R, $q = Q/m_{\mathrm{e}}c^2$, and the spectral shape factors $S_{(m)x}$ to lowest order are given by

$$S_{(m)x} = \begin{cases} 1 & \text{for } m = \mathrm{a},\ \mathrm{nu} \text{ and } x = n\mathrm{s}_{1/2},\ n\mathrm{p}_{1/2} \\ q^2 & \text{for } m = \mathrm{u} \text{ and } x = n\mathrm{s}_{1/2},\ n\mathrm{p}_{1/2} \\ 9/R^2 & \text{for } m = \mathrm{u} \text{ and } x = n\mathrm{p}_{3/2},\ n\mathrm{d}_{3/2} \\ 0 & \text{otherwise}^{\dagger}. \end{cases} \tag{16}$$

† This choice was done so as to be consistent with the use of terrestrial *ft* values in eq. (13). In the bound-state β^- transition between ionic ground states, it may happen that the Pauli principle forbids the creation of an electron in those low-spin states. This conflict is, however, not severe in calculating the *total* rates as they are usually determined by dominant contributions from the insertions of low-spin electrons either into the single-particle hole states found in low-lying ionic excited-states or into the next empty major shell.

A complexity arises in connection with electron (or positron) wave functions in stellar interiors. In particular, the evaluation of the screening effects due to the bound electrons and perturbers is cumbersome, since the decaying electron (or positron) feels different fields depending on the ionic states.

The continuum-state electron (or positron) wave functions corrected for the screening effects that are caused by the orbital electrons are approximately evaluated for given momenta by linear interpolation (as a mere function of the total number of the bound electrons) between the values obtained for the neutral atom [35]) and the well-known values for the point-charged bare nucleus [36]). Dealing with densities that are not extremely high, we neglect the expected small screening effects that are due to perturbers. The screened orbital-electron wave functions, on the other hand, are directly obtained by the method of Liberman *et al.* [25]), under the assumption that the perturbers do not change the wave functions appreciably. This assumption may be partly supported by the approximate constancy of the perturbing potential inside the ion. The electron configurations are taken to be those of the ionic ground-states, this saving computational time without significant loss of accuracy.

The imperfect overlap of the atomic wave functions and exchange effects [37]) on the transition rates are expected to be small in heavy nuclei [38]), and are disregarded here.

3.2.3. Total β-transition rates. The Kth excited state of nucleus i decays with the effective rate given by

$$\lambda_{i(K)} = \sum_j n_{ij}\lambda_{i(K)j} \Big/ \sum_j n_{ij} , \tag{17}$$

with

$$\lambda_{i(K)j} = \left[\sum_{K'kk'} b_{ijk} \exp\left(-e^*_{ijk}/\kappa T\right) \lambda_{\mathrm{IF}}^{(m)} \right] \times \left[\sum_k b_{ijk} \exp\left(-e^*_{ijk}/\kappa T\right) \right]^{-1} , \tag{18}$$

where m specified by K and K' is either a, nu or u as described before.

If the nuclear levels are in thermal equilibrium, the total decay rate of nucleus i is given by

$$\lambda_i = \sum_K \left[G_{iK} \exp\left(-E^*_{iK}/\kappa T\right) \lambda_{i(K)} \right] \Big/ \sum_K G_{iK} \exp\left(-E^*_{iK}/\kappa T\right) , \tag{19}$$

with G_{iK} being the spin weight of the Kth initial nuclear level. This formula is appropriate in most cases, except eventually in some nuclei with long-lived isomeric states. In these cases, the equilibration time-scale may be comparable to or even longer than the time-scales of other nuclear reactions and/or of changes in astrophysical conditions. If so, eq. (19) should be disregarded. Instead, the summation over the nuclear levels K should be taken according to their populations which

vary with time as a result of nuclear excitations, de-excitations and destructive mechanisms following the precursory reaction [39]).

4. Numerical examples and discussion

The significance of the present formalism may be most directly realized in the bound-state β^- decay and orbital-electron capture processes, and in particular those with low transition energies. This is shown in the following by way of a few selected examples.

4.1. BOUND-STATE β^- DECAYS

(i) Cosmochronological importance – ^{187}Re case. This nucleus is known to undergo a unique first-forbidden β^- transition to the ground state of ^{187}Os, its half-life being $(4.28 \pm 0.08) \times 10^{10}$ y [ref. [40])]. Because of this long half-life, the ^{187}Re–^{187}Os pair has been considered as one of the most promising cosmological clocks [41]). A question then raised was whether the ^{187}Re decay rate could be enhanced in stellar interiors [42]). In fact, judging from the energetics, one expects such an enhancement as the result of bound-state β^- decays of highly ionized ^{187}Re atoms.

Indeed, a few attempts have been made [17,18]) to answer that question. Mainly from Perrone's rates [17]), it has generally been considered that the enhancement effect would not reset the clock [43]). However, this conclusion is highly questionable since the possibility of a non-unique bound-state β^- transition from the ^{187}Re ground state to the 9.75 keV first excited state of ^{187}Os has been overlooked in those studies [17,18]). We have briefly reported [19]) some results which demonstrate that, owing to this neglect, the calculations by Perrone [17]) greatly underestimate the ^{187}Re decay rate in stellar interiors. Because of its astrophysical importance, and because of the fact that this is one of the most delicate cases in which our present formalism should be successfully applied, we consider it worthwhile to go into further details here.

For the sake of simplicity, we restrict the following discussion to the nuclear levels shown in fig. 1, which are of primary importance at relatively low temperatures as in the interiors of main-sequence stars. [Even for typical s-process temperatures

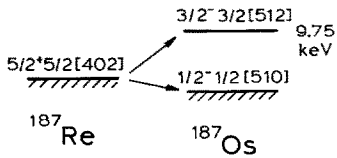

Fig. 1. Nuclear levels of major importance in ^{187}Re bound-state β^- decays.

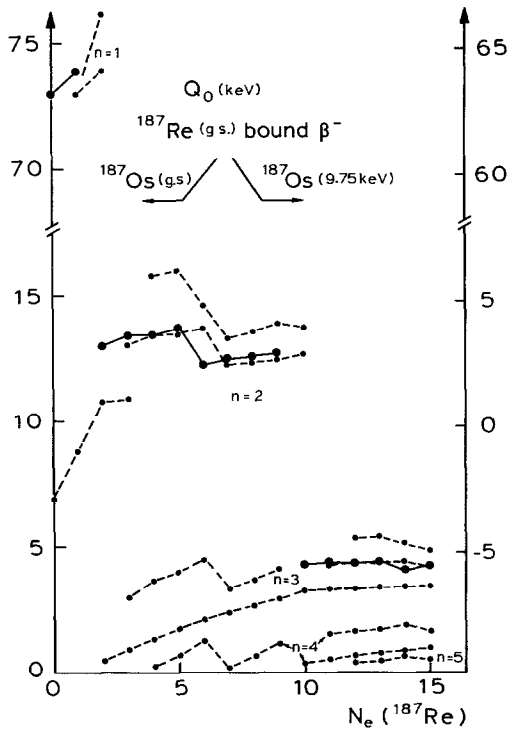

Fig. 2. Q-values of bound-state β^- decays of highly-ionized ^{187}Re in the absence of the continuum depression. $N_e(^{187}\mathrm{Re})$ is the number of electrons bound to ^{187}Re and n is the principal quantum number of the electron to be created. The left- (right-) hand side scale refers to the unique (non-unique) first-forbidden transition feeding the ^{187}Os nuclear ground (9.75 keV excited) state, respectively. Full lines connect the values for the ionic ground-ground transitions and the dashed lines the values for the transitions that involve the ionic excited states as initial and/or final states.

($\sim 3\times 10^8$ K), the inclusion of other levels has only a minor effect on the total transition rate.] The Q_0 values [i.e. Q-values in absence of continuum depression effect; eq. (10b)] for the bound-state β^- decays of the ^{187}Re nuclear ground state are displayed in fig. 2 as a function of the number of the electrons that are bound to ^{187}Re. The ionic ground-state energies are calculated self-consistently [25]), while the ionic excitation energies are derived from a schematic hydrogen-like model introduced in appendix B. The real Q-values are given by $Q = Q_0 - \Delta_{75}$ [eq. (12)], Δ_{75} being the continuum depression correction. Clearly, the bound-state β^- decay of ^{187}Re into the 9.75 keV ^{187}Os level is energetically possible as long as the degree of ionization is high (i.e. if the number of orbital electrons is less than ~ 10) and Δ_{75} is comparatively small. If this is the case, the non-unique first-forbidden transition may give an overwhelming contribution to the ^{187}Re decay rate, non-unique transitions being usually much faster than unique ones. [Note that the transitions to the higher excited states of ^{187}Os are either almost negligible or

energetically forbidden. The Q-value for the continuum-state β^- decay of ^{187}Re to the ^{187}Os ground state is at a maximum 2.64 keV if the atom is neutral and goes down to negative values in highly ionized cases ($\simeq -12.7$ keV for full ionization).]

The total β^- decay half-life of 4.3×10^{10} y of neutral ^{187}Re and the neutral atomic mass difference of 2.64 keV lead to the $\log(f_1 t) = 11.0$ for the unique ground–ground transition. This value can be practically considered as that of the continuum-state β^- decay which is required in eq. (13). [See ref. [44]) for a discussion of the possibly small bound-state β^- decay contribution to the total decay rate of neutral ^{187}Re.] The $\log(f_0 t)$ value for the non-unique transition, which is important to determine the absolute decay rate of ^{187}Re, is taken to be 7.5 after a survey of the reduced nuclear matrix elements of transitions observed between the $\frac{5}{2}^+\frac{5}{2}$[402]p and $\frac{3}{2}^-\frac{3}{2}$[512]n Nilsson states [45]).

The relevant radial wave functions of the electrons inserted in ^{187}Os orbits are evaluated at the nuclear radius of $1.2 \times A^{1/3}$ fm by the method described in subsect. 3.2.2, with the results partly shown in fig. 3.

The calculated ^{187}Re bound-state β^- decay rates are presented in fig. 4. The tremendous deviations of the total rates (solid curves) from the partial rates of the unique transition to the ^{187}Os ground state (dashed or dotted curves) clearly indicate the importance of the non-unique transition to the 9.75 keV excited state in stellar interiors. Further results and their implications for the ^{187}Re–^{187}Os chronology in the framework of a model for the chemical evolution of the Galaxy in the solar neighborhood have recently been discussed in detail in ref. [22]). [The calculation of the transmutation rates between ^{187}Re and ^{187}Os in stellar interiors, which is requested in chronological studies, is complicated by the possible electron captures of ^{187}Os; see ref. [46]). Furthermore, such rates under s-process conditions are also requested in the evaluation of the s-process component of ^{187}Os when due care is taken of the branchings in the $A = 185$–187 region [47]).]

(ii) Importance in the s-process – ^{163}Dy case. The stellar β-decay rate of this terrestrially stable element has been studied in attempts to explain the ^{164}Er solar abundance (which is an order of magnitude greater than those of the p-process elements in this mass region) in terms of an s-process branching. The scenario [20]) for producing an s-process component of ^{164}Er starts with the β^- decays of the thermally populated excited states (particularly, one at 73.4 keV) of ^{163}Dy, followed by the successive reactions ^{163}Ho(n, γ)^{164}Ho(β^-)^{164}Er. In the meantime, the thermal pulse stage of intermediate mass stars was suggested to be a promising site for the s-process [48]). If this is the case, the above scenario might become doubtful [49]): in the absence of neutrons during the interpulse period, the very β-decay product ^{163}Ho would capture free and orbital electrons back to the groundstate of ^{163}Dy. In addition, due to the relatively low temperatures expected in the interpulse period, the thermal population of the excited state would be less effective than in the pulse period. Then, the net effect might be such that there would be almost no ^{163}Ho awaiting the next pulse to capture neutrons.

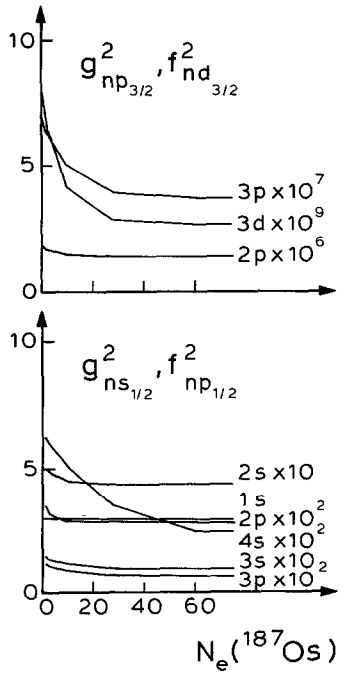

Fig. 3. The squared larger components of electron radial wave functions in ^{187}Os (N_e being the number of bound electrons) evaluated at the nuclear surface. The results, shown for some lowest n-values, are obtained by the method of Liberman *et al.* [25]) for the lowest energy configurations.

In the following, these arguments are reconsidered, noting the possibility of bound-state β^- decay of the ^{163}Dy *ground* state. This transition has never been considered, in spite of the fact that it may be fast enough to lead to ^{164}Ho during the pulse period, or to force some ^{163}Ho to survive the interpulse period. [Joukoff [15]) claimed the importance of the bound-state β^- decay of the 73.4 keV level. However, its effect has generally been overestimated as a result of a numerical mistake.]

The nuclear levels of importance in "typical" s-process temperatures are displayed in fig. 5. The half-life, and thus the log (f_0t) value of the ground-state ^{163}Ho decay (to the ground state of ^{163}Dy), is hitherto unknown experimentally [50,51]). A study of the reduced nuclear matrix elements [corrected for the pairing effect [52])†] between the $\frac{7}{2}^-\frac{7}{2}$[523]p and $\frac{5}{2}^-\frac{5}{2}$[523]n Nilsson states in this mass region implies that the log (f_0t) value is most likely 5.0 ± 0.2. Adopting this value and taking into account the appropriate Clebsch–Gordan coefficients, we obtain the relevant log (f_0t) values of β^- decays of the ^{163}Dy levels into the ^{163}Ho levels. With respect to the neutral atomic mass difference between those isobars, a recent measurement [50]) gives 2.3 ± 1.0 keV, while the measured partial half-life $(4.0 \pm 1.2) \times 10^4$ y

† In ref. [50]), the pairing correction factors of the ^{161}Ho and ^{163}Ho decays are reversed.

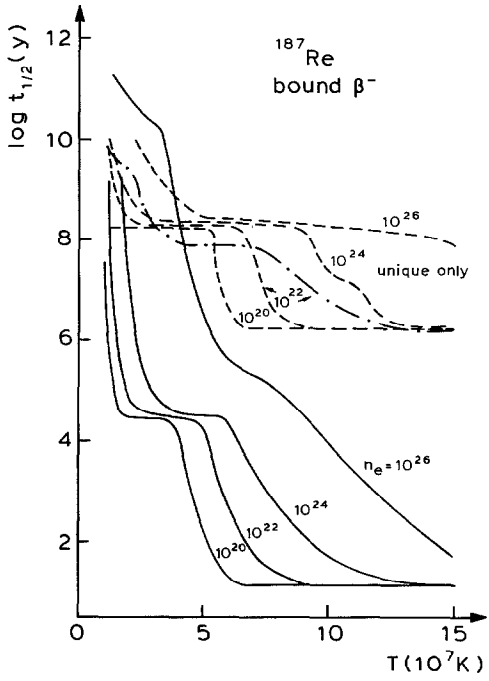

Fig. 4. ^{187}Re bound-state β^- decay half-lives calculated for various temperatures T and electron number densities n_e (per cm^3). Solid curves present the total half-lives, while the partial half-lives of the unique transition are shown by dot-dashed [present work] and dashed [ref. [17])] curves.

of the ^{163}Ho M electron capture [50]) combined with the above-adopted log $(f_0 t)$ value suggests 2.6 ± 0.2 keV in the case of the massless neutrino. Fortunately enough, the uncertainty of the order of 1 keV in the energetics does not cause serious trouble in our present study. Under s-process conditions, the ^{163}Dy atoms are indeed so highly ionized that the bound-state β^- decays to the unoccupied K- or at least L-shells contribute dominantly to the total decay rate. [As mentioned before, the ^{163}Ho electron captures are as important as the ^{163}Dy decays in the ^{164}Er problem. But, once again, small energy changes do not matter so much since the Q-values become of the order of 10 keV in s-process conditions.]

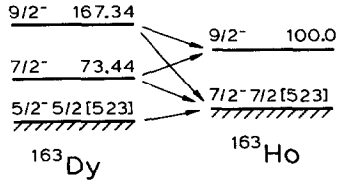

Fig. 5. Nuclear levels relevant for the calculation of the bound-state β^- decay rates of ^{163}Dy in s-process conditions. The excitation energies are in keV.

The calculated total β^- decay rates of ^{163}Dy embedded in a pure He matter are displayed in fig. 6 as a function of temperature, the density being $\rho = 3 \times 10^3$ g/cm^3. The importance of the bound-state β^- decay of the ^{163}Dy ground state is now apparent. Further results will be reported elsewhere in conjunction with the ^{164}Er problem.

4.2. ORBITAL e^- CAPTURES

(i) Low-energy transitions. From the above, it is clear that orbital e^- captures as the inverse process of bound-state β^- decays should be treated with some care whenever the transition energies are expected to be comparable with the energy changes caused by ionization. An apparent example concerns the e^- captures by the thermally populated 9.75 keV excited state of ^{187}Os, which is energetically possible if the degree of ionization is not extremely high (cf. fig. 2). In this case, which may be realized in the interiors of low-mass main-sequence stars, the e^- captures compete with, and may even overcome, the unique bound-state β^- decay of ^{187}Re. The cosmochronological consequences of such a situation are discussed in ref. [22]).

(ii) High-energy transitions. It is of interest to show that orbital e^- capture rates can be rather accurately calculated by a simpler approach when the transition energies are high enough so that the K-electron captures are dominant: namely, the so-called Strömgren formula [53]) may be applied to calculate the average numbers N_n of electrons in orbits with principal quantum numbers n, which reads

$$N_n = 2n^2/[1 + \exp(-X_n/(\kappa T) - \eta)], \tag{20}$$

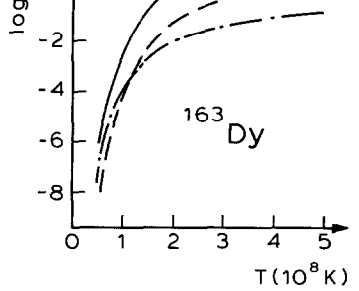

Fig. 6. Calculated β^- decay rates of ^{163}Dy embedded in a pure He matter at density $\rho = 3 \times 10^3$ g/cm^3 as a function of temperature T. The relevant $\log(f_0 t)$ values are obtained by assuming $\log(f_0 t) = 5.0$ for the ^{163}Ho ground-state decay, and the neutral atomic mass difference is taken to be 2.3 keV (see text). The major contribution to the total decay rate of ^{163}Dy (solid curve) comes from the bound-state β^- decays of its ground state, while minor contributions come from the decays of the excited states by the bound- (dashed curve) and continuum- (dot-dashed curve) state β^- decays.

where $X_n = \mathrm{Ry}\, Z^2/n^2$ with Ry being the Rydberg unit of energy. These values are to be compared with those obtained by solving the Saha equation with due consideration for the electron configurations of the ionic ground as well as excited states. Such a comparison is made in table 1 for Ho as an example. The good agreement for the K-shell ($n = 1$) N_K values indicates the validity of the Strömgren formula in the calculations of high-Q-value orbital e^- capture rates of such heavy elements. For instance, the resulting capture rates of ^{164}Ho (the neutral atomic mass difference being 1.03 MeV) deviate from those obtained with the Saha equation by no more than 10% in wide ranges of T and ρ if the same electron wave functions are used in both cases.

4.3. CONCLUDING REMARK

In this paper, we have re-investigated β-transitions of highly ionized heavy atoms in stellar interiors with emphasis on the ionic effects in the case of low-energy transitions at rather high temperatures and not extremely high densities. A systematic study of such transitions is called for in connection with, among others, s-process

TABLE 1

Calculated K- and L-shell occupation numbers, N_K and N_L, of Ho embedded in a pure He matter at various temperatures T (in 10^8 K) and densities ρ (in 10^3 g/cm^3) [note the overall good agreement of N_K values calculated by the Strömgren formula [53]) with the present results obtained from the Saha equation]

T	ρ	N_K		N_L	
		Strömgren	Saha	Strömgren	Saha
1	1	1.973	1.964	2.131	1.648
	3	1.991	1.996	4.253	3.082
	10	1.998	2.000	6.512	4.892
1.5	1	1.574	1.577	0.771	0.554
	3	1.838	1.890	1.973	1.484
	10	1.952	1.977	4.328	3.177
2	1	0.838	0.851	0.385	0.135
	3	1.374	1.431	1.067	0.682
	10	1.770	1.820	2.802	2.048
3	1	0.209	0.217	0.155	0.065
	3	0.521	0.533	0.452	0.159
	10	1.092	1.252	1.359	0.672
4	1	0.078	0.081	0.085	0.045
	3	0.218	0.219	0.251	0.104
	10	0.586	0.600	0.792	0.302
5	1	0.039	0.040	0.054	0.034
	3	0.112	0.113	0.161	0.081
	10	0.335	0.328	0.520	0.217

branching problems in attempts to constrain s-process models. In particular, the roles played by bound-state β^- decays deserve careful attention in case studies. Examples of this kind may concern nuclei such as ^{93}Zr, ^{107}Pd, ^{151}Sm, ^{155}Eu, ^{157}Gd, ^{171}Tm, ^{179}Hf, ^{191}Os, ^{195}Pt and ^{205}Tl in addition to the above-discussed ^{163}Dy and ^{187}Re.

The authors' special thanks go to Marcel Arnould who drew their attention to most of the problems dealt with in the present paper, particularly for his providing them with several unchallenged references. They should like to express their sincere thanks also to Eberhard Hilf, without whose deep interest and warm and unselfish support this work could not have been completed. The required numerical calculations have been performed on the IBM-3032 at the Gesellschaft für Schwerionenforschung, Darmstadt. The financial supports by this institution and by the Deutsche Forschungsgemeinschaft are highly appreciated.

Appendix A

CONTINUUM DEPRESSION EVALUATED FROM A FINITE-TEMPERATURE THOMAS–FERMI MODEL

In an attempt to evaluate the continuum depression (subsect. 2.2), Stewart and Pyatt [23]) have studied the perturbing potential due to the surrounding free electrons and neighboring ions within the framework of a finite-temperature Thomas–Fermi model.

The first step is to consider a nucleus with charge Ze fixed at the center of a sea of electrons (bound plus free) and neighboring point ions (with expected small influence of neutral atoms, and positrons being neglected). Then, the total potential distribution $\Phi(r)$, assumed to be spherically symmetric, follows a Poisson equation

$$r^{-1}\,\mathrm{d}^2(r\Phi)/\mathrm{d}r^2 = -4\pi e\left[\sum_{ij} j n_{ij}(r) - n_e(r)\right], \tag{A.1}$$

where the local number density of non-relativistic, non-degenerate ions $n_{ij}(r)$ and of electrons $n_e(r)$ are given by

$$n_{ij}(r) = n_{ij}(\infty)\exp\left(-je\Phi/\kappa T\right), \tag{A.2}$$

$$n_e(r) = n_e(\infty)F(e\Phi/\kappa T + \eta, \beta)/F(\eta, \beta), \tag{A.3}$$

with the asymptotic number densities $n_{ij}(\infty)$ and $n_e(\infty)$, which correspond to those discussed in subsect. 2.1 and satisfy the charge neutrality $\sum_{ij} j n_{ij}(\infty) = n_e(\infty)$. The boundary conditions for eq. (A.1) are $\Phi(\infty) = 0$ and $\Phi(r) \to Ze/r$ as $r \to 0$. In terms of the dimensionless quantities

$$y = e\Phi/\kappa T, \qquad x = r/D, \qquad D^{-2} = (4\pi e^2/\kappa T)\sum_{ij}(j^2 + j)n_{ij}(\infty), \tag{A.4}$$

eq. (A.1) reads

$$x^{-1}\,\mathrm{d}^2(xy)/\mathrm{d}x^2 = [F(y+\eta,\beta)/F(\eta,\beta) - \langle \exp(-jy)\rangle]/(1+\langle j\rangle)\,, \tag{A.5}$$

with the definition

$$\langle X\rangle = \sum_{ij} X j n_{ij}(\infty) \Big/ \sum_{ij} j n_{ij}(\infty)\,. \tag{A.6}$$

As described in ref. [23]), the second step is to extract the effects that are due to perturbers. The perturbing potential Φ_{p}, created by the free electrons and neighboring ions, is described as

$$x^{-1}\,\mathrm{d}^2(xv)/\mathrm{d}x^2 = S(x)\,, \tag{A.7}$$

in terms of

$$v = e\Phi_{\mathrm{p}}/\kappa T\,, \tag{A.8}$$

$$S(x) = [G(y+\eta,\beta,y)/F(\eta,\beta) - \langle \exp(-jy)\rangle]/(1+\langle j\rangle)\,, \tag{A.9}$$

where

$$G(y+\eta,\beta,y) = \int_{1+y/\beta}^{\infty} W(W^2-1)^{1/2}[1+\exp(\beta(W-1)-\eta-y)]^{-1}\,\mathrm{d}W\,. \tag{A.10}$$

In the above, the "free electrons" are defined as those electrons with kinetic energies exceeding $e\Phi$. A choice of the zero of the potential such that $v(\infty)=0$ gives

$$v(x) = -x^{-1}\int_0^{\infty} S(z)z^2\,\mathrm{d}z + x^{-1}\int_x^{\infty} S(z)z^2\,\mathrm{d}z - \int_x^{\infty} S(z)z\,\mathrm{d}z\,. \tag{A.11}$$

Noting that, at large x, $y(x)-v(x)$ has an asymptotic Coulomb form which depends only on the net ionic charge and $y(x)$ vanishes exponentially, one gets the net ionic charge (after ionization), $(j+1)e$, from

$$(j+1)e^2/(D\kappa T) = \int_0^{\infty} S(z)z^2\,\mathrm{d}z\,. \tag{A.12}$$

As expected, the perturbing potential depends strongly on densities. For a not extremely high ($\lesssim 10^4$ g/cm^3) density, however, its radial dependence is weak up to large distances. Because of this near constancy, the lowering of the ionization potential can be well approximated by $-v(0)\kappa T$, except for the removal of an electron from outer orbits: namely, Δ_{ij} in eq. (7) is replaceable by

$$\Delta_j \equiv -v(0)\kappa T = \kappa T\int_0^{\infty} S(z)z\,\mathrm{d}z\,, \tag{A.13}$$

as suggested in ref. [23]).

Let us now consider a heavy nuclear species embedded as a tiny remainder in hydrogen- and/or helium-dominant matter at temperatures $T \simeq 10^6$–10^9 K and

densities $\rho \simeq 10^{-4}$–10^{4} g/cm^3. These conditions are commonly realized over a long time interval during stellar evolution. Under such circumstances, hydrogen and helium are almost fully ionized. Therefore, the iterative solutions of the coupled Saha and Thomas–Fermi equations converge very quickly and are almost independent of the assumed tiny amount of the remainder. This situation enables us to express the continuum depression Δ_j as a mere function of the temperature T, free electron number density n_e and net ionic charge j. The numerical results can be approximated as

$$\log \Delta_j(\mathrm{keV}) = [d_1 \log T_7 + d_2] \log (j+1) + [d_3 (\log T_7)^2 + d_4 \log T_7 + d_5], \quad \text{(A.14)}$$

where T_7 stands for T in 10^7 K, and

$$\begin{aligned} d_1 &= 0.00135(\log N)^2 - 0.0002(\log N) + 0.01, \\ d_2 &= -0.00297(\log N)^2 + 0.00563(\log N) + 0.99, \\ d_3 &= -0.000518(\log N)^2 - 0.0058(\log N) + 0.001, \\ d_4 &= 0.00358(\log N)^2 + 0.000297(\log N) - 0.5, \\ d_5 &= -0.00445(\log N)^2 + 0.5171(\log N) - 4.658, \end{aligned} \quad \text{(A.15)}$$

with $N = n_e$ (in cm^{-3})$/(5.2 \times 10^{18})$ [for example, $N = 10$ and 10^9 correspond respectively to $\rho = 10^{-4}$ and 10^4 g/cm^3 for the composition $x_H \simeq 0.75$ and $x_{He} \simeq 0.25$]. This approximation results in less than $\pm 10\%$ errors in Δ_j.

It should be emphasized here that the above procedure for obtaining Δ_j and the cut-off method (subsect. 2.2) were introduced merely as useful tools for tackling the problems dealt with in the present paper. Therefore, one has to be cautious if Δ_j becomes of the order of uncorrected ionization potential I_{ij}. This appears to be the situation at high ρ and low T, in which slight errors in Δ_j lead to considerably different solutions of the Saha equation.

Appendix B

SCHEMATIC MODEL OF IONIC EXCITED STATES

As mentioned in subsect. 2.2, it is very time consuming to calculate the excitation energies of ionic states in a self-consistent way [25]). Here, we construct a schematic model of ionic excited states in order to simplify the equilibrium calculation, and confront the resulting ionic abundances with those obtained by using the self-consistent ionic levels.

The first simplification is to assume single-particle electrons filling up the orbits according to the serial order of the principal quantum number n and of the orbital quantum number l. This assumption seems to be reasonable as long as the degree of ionization is high [54]). Then the ground-state configuration can be specified by

the quantum numbers n_0 and l_0 of the last electron and the number of electrons $N(n_0 l_0)$ in this orbit. The total number of electrons in the major n_0 shell is $N(n_0) = 2l_0^2 + N(n_0 l_0)$. If $N(n_0) \neq 2n_0^2$ and $n_0 \neq 1$, those $N(n_0)$ electrons can have configurations other than that of the ground state within the same n_0 shell. We regard them as the first-excited-state configurations and assume that all of them are energetically degenerate. Similarly, we construct higher excited states by excitations of single electrons from the n_0 shell into the higher major shells $n(>n_0)$ without bothering about the energy differences between the subshells. Within this simple model, the statistical weights b_{ijk} are given by

$$b_{ijk} = \begin{cases} C[2(2l_0+1), N(n_0 l_0)] & \text{for } k = 0 \text{ (g.s.)} \\ C[2n_0^2, N(n_0)] - b_{ij0} & \text{for } k = 1 \\ 2(n_0+k-1)^2 C[2n_0^2, N(n_0)-1] & \text{for } k \geq 2\,, \end{cases} \tag{B.1}$$

where $C[s,t] = s!/[t!(s-t)!]$.

Furthermore, we approximate the excitation energies of these levels by

$$e^*_{ijk} = I_{ij} - \mathrm{Ry}\,(j+1)^2/(n_0+k-1)^2\,, \tag{B.2}$$

for $k \geq 1$ if $b_{ij1} \neq 0$ and for $k \geq 2$ if $b_{ij1} = 0$, where I_{ij} is the ionization potential and Ry represents the Rydberg unit of energy. This result is obtained by applying the classical hydrogen-like formula to the last electrons which are in $n = n_0 + k - 1$ major shells, and are assumed to feel the net charge $(j+1)e$.

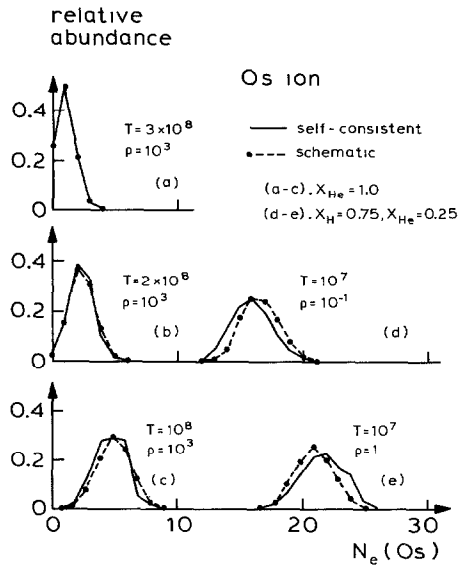

Fig. 7. Relative abundances of Os ionic states (N_e: the number of bound electrons) from the Saha equation for various sets of temperature T(K), density ρ(g/cm^3), and hydrogen and helium mass fractions, x_{H} and x_{He}. The solid lines connect the values with the ionic data obtained by the self-consistent field method [25]), and the dashed lines the values derived from the schematic model described in appendix B. The same cut-off energies Δ_j are used in both cases.

The above model, combined with the *ad hoc* assumption of cut-off by Δ_j, is certainly very crude for calculating individual atomic partition functions. Fortunately, however, the present study requires mostly the ratios of partition functions as in the Saha equation (1). The solutions of the Saha equation with the use of the partition functions obtained above and those obtained by the self-consistent method [25]) are compared in fig. 7 for Os. The agreement, and hence the applicability of the above schematic model, is considered as quite satisfactory, at least in the present state of the art.

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