Optical Properties of Plasmas of High-Z Elements

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1. Introduction

The optical properties of tungsten were presented in the previous works [1,2]. In this works, the spectra were investigated with taking into account the electrostatic and spin-orbital splitting of the unfilled shells of equivalent electrons. The interaction of two unfilled shells was also taken into account. In this case, the linear transitions between two configurations are splitted into a large number of components. The validity range of these results is limited by the temperature up to $T \approx 20 \text{ eV}$. Such a temperature restriction is depends on a number of reasons. The approach of local thermodynamic equilibrium (LTE) was used in these
calculations. This approach limits the validity range of model in the temperature. The method taking into account the splitting in spectra is limited by the $d^q$ and $p^q$ configurations, where $q$ is the number of electrons in configuration. At temperatures higher than 20 eV the $4f^q$ configuration is occurred. In the given work the collisional radiative equilibrium model (CRE) was developed with the account of the electrostatic and spin-orbital splitting for the unfilled $p^q$, $d^q$ and $f^q$ shells [3]. Thus, the given model has no restrictions on the validity in temperature and density. Below the detailed theory to take into account the splitting is presented.

Below in Sec. 2 the problems associated with account of the electrostatic and spin-orbital splitting in an atom are discussed. Various typical radiative transitions are considered. Some results of calculations in the LTE approximation and a comparison with data of other authors are presented. The theory for calculation of thermodynamic and optical characteristics of the heavy elements in the CRE approximation is discussed in more details and numerous results are shown in Secs. 3-7. The model is applicable for the unfilled $p$, $d$ and $f$ shells. In Sec. 8, the statistical theory of radiation transfer applicable for complex spectra of the heavy elements is presented. Radiation fluxes calculated in spectral and statistical Lebesgue approximations are compared.

### 2. Calculation of Optical Properties of Tungsten Plasma in LTE Approximation

In the LTE approximation, the collisional processes (excitation and ionization) are only taken into account. All the radiative transitions are treated as negligible small and are not taken into consideration. The validity range of this approximation is limited by high densities and low temperatures. In our calculations, the upper temperature boundary was chosen about 20 eV. At the first stage, the calculations of optical properties were carried out in the LTE approximation with the account of the splitting for the $p$ and $d$ shells. In this case, the structure of levels can be calculated with use of the perturbation theory. As the basis, the energy levels and wave functions obtained in the HFS or HF approximation for the average term are taken. Further, using these wave functions the magnitude of electrostatic splitting for the total set of $L,S$ quantum numbers and also the spin-orbital splitting for all quantum numbers of the total moment $J$ are calculated. The theory to calculate these splittings is relatively simple for the
unfilled $p^q, d^q$ shells, but is very complex for the $f^q$ shells. At the first stage, the $p^q, d^q$ shells were only considered. The determined structure of levels is used to calculate the ionization plasma balance and the populations of levels. In the LTE approximation the problem is reduced to the solution of the Saha equations

$$\frac{N_{i+1} N_i}{N_i} = 2 \frac{U_{i+1}}{U_i} \left(\frac{m_i k T}{2 \pi h}\right)^{3/2} \exp\left(\frac{I_i}{k T}\right).$$

Here, $N_i, N_{i+1}$ are the concentrations of $i$–th and $i+1$–th ions, $U_i, U_{i+1}$ are the statistical sums of corresponding ions determined by the expression

$$U_i = \sum_{M=1}^{M_{\text{eq}}} g_M \exp(-E_M / k T),$$

where $g_M$ is the statistical weight of the level $M$, $E_M$ is the level energy, $I_i$ is the ionization potential of $i$-th ion, $T$ is the plasma temperature.

### 2.1. Features and Assumptions for Calculation of Optical Properties of Tungsten Plasma

To solve some applied problems the knowledge of thermodynamical and optical properties of construction material plasmas (for instant tungsten, iron, titanium, etc) is required. To calculate the optical properties of these elements in the LTE approximation it is necessary to take into account some features, which are listed below.

- The self-consistent Hartree-Fock (HF) or Hartree-Fock-Slater (HFS) calculation methods become more complex for heavy elements because of the great number of electrons. The presence of unfilled $d$ and $f$ shells leads to decreasing of accuracy and increasing of iteration numbers.
- For the heavy elements, the spin-orbital and electrostatic splitting can not be neglected in the calculations. In some cases, the magnitude of the electrostatic splitting can exceed half an ionization potential from the ground state. In this case, all the atomic levels have to be calculated independently with the procedure of self-consistency being performed for each level.
- As the available experimental data on the atomic structure for the heavy elements are fragmentary, the semi-empirical methods can not be used to calculate the optical properties. It is also impossible to identify spectra of the heavy elements.
- Significant difficulties appear when the plasma models (for example CRE) are used for the heavy elements because a lot of energy levels should be taken into account. For the heavy elements the dimensionality of the kinetic equation system, which have to be solved, increases significantly. A lot of multipole and
intercombinative transitions, which are neglected for the light elements, should be taken into account also. Rates of these transitions are not fully investigated and methods for calculations of them are only estimating with low accuracy. In some cases such processes as impact excitation and ionization through auto-ionized levels, double auto-ionization should be taken into account also.

- There are a lot of splitted spectral lines in the spectra of the heavy elements, which leads to significant difficulties in radiation transfer calculations.

Therefore, the self-consistent method can not be directly used to calculate the atomic structure of the heavy elements as well as the CRE model to calculate the optical properties. In this case, some assumptions and simplifications of the models are done to decrease the amount of calculations. Below the used assumptions are listed.

♦ The spin-orbital and electrostatic splitting are fully neglected. The atomic structure is calculated using either the HFS method in the configuration assumption or the HF method in the average ion assumption. (Both methods give the same results). In this case, the specter consists of the isolated strong lines, which are the sum of splitting components. This specter is similar to the light element one. It should be noted that such a model is a rough approximation and can be used for multi-ionized ions where the splitting is not so large. However, the use of these optical properties in the radiation transfer calculations can lead to rough mistakes.

♦ The next approximation is the statistical method, which takes into account the splitting [4,5]. In this method, the atomic structure is calculated either for the average term or for the configuration with the splitting width being estimated. Further, it can be assumed that line components are set out within the splitting width and are distributed in accordance with the normal law. Its relative intensities are also distributed in accordance with the normal law. The integral over the counter of the set of lines is equal to the line strength obtained using the average ion assumption. In effect, the group of line components is changed by the single line with the effective width being close to the splitting width. This model is valid if a number of line components is large and the intensities of components correspond really to the normal law. Additionally, the distances between components have to be comparable with the line width, otherwise the averaged coefficients will be calculated with a low accuracy, for example, mean Rosseland coefficients will be overestimated. The reference data [6] confirm this conclusion. Using of this method is restricted by the $f^q$ terms with $4 < q < 10$.

♦ The next approximation is the development of previous model for the $p$ and $d$ shells as well as for the $f$ shells having a low number of electrons or for the closed $f$ shells. In this case, the atomic structure is calculated using the average term approximation, but the splitting width and intensities of the
components are obtained directly using the quantum numbers of each component and the Racah techniques. Further, each component is taken, as an isolated line having own width and the specter is the sum of all the components. This method is more complex then previous one but the mean Planck and Rosseland coefficients are obtained with a good accuracy. Authors developed the effective procedure to calculate all the above-mentioned characteristics and specter construction. This method was used to calculate the absorption and emission coefficients of the tungsten plasma.

2.2. Spin-Orbital and Electrostatic Splitting

In this item in the LTE approximation the electrostatic and spin-orbital splittings are considered for the $p^q$ and $d^q$ shells of the heavy elements. The $f^q$ shells are not taken into account. The electrostatic splitting is determined by the dependence of energy on the total orbital $L$ and total spin $S$ momenta.

The HFS method in the configuration approximation is used to calculate the energy levels and wave functions. In this approximation only one level, which is independent on the $L, S$ quantum numbers of the term, corresponds to each configuration, for example, to the ground state $5d^{4}6s^{2}$ of the tungsten atom.

Tungsten has the large charge number $Z = 74$, therefore the relativistic correction should be taken into account. In our model, the perturbation method with the non-relativistic HFS wave functions is used to calculate the relativistic corrections. All the main relativistic effects, mass-dependence on velocity, contact and spin-orbital electron interactions, were taken into account. A comparison with detailed Dirac-Fock calculations shows a satisfactory accuracy of this method.

Thus, energy levels and wave functions are calculated using the configuration approximation. The wave functions can be used to calculate the different integrals which does not contain the angle variable, for example, matrix elements required to calculate the oscillator strengths, photo-ionization cross sections, broadening constants, etc. For example, the direct and exchange $F^{k}$ and $G^{k}$ Slater integrals determining the electrostatic splitting scale as well as the constant $\xi_{nl}$ of the spin-orbital splitting are very important. Expressions to calculate these characteristics will be presented in Sec. 3.

Beside these characteristics, the splitting width depends significantly on angle characteristics. Both the set of quantum numbers of terms and the genealogical structure of terms determine the angle characteristics. In this case, the numerical factor before the integrals is the complex algebraic expression consisting of $3nj$-symbols and genealogical coefficients. $3nj$-Symbols allow us to calculate the total momentum as a sum of the several momenta. The genealogical coefficient determines the probability of term formation when one electron is removed from the shell.

There are direct and exchange angle coefficients too. They depend significantly on the orbital quantum number $l$ and a number of equivalent electrons in the shell as well as whether an interaction is considered within the
shell or between different shells. There are a lot of expressions for all the cases. Because of an inconvenience of them, we don't list these expressions.

In the practical problems all the above mentioned situations are realized. Let us take tungsten as an example.

Line transitions of tungsten can be classified as follows

1. The transition from the ground state \( 5d^46s^2 - 5d^46s6p \).

   There are unfilled inner shell \( 5d^4 \) and closed outer shell \( 6s^2 \) in the ground state. In this case, the interactions between the groups of \( d-d \), \( s-s \), \( s-d \) electrons are calculated. Each of these transitions produces the own splitting structure and the resulting splitting is its superposition. The excited configuration has the following electron interactions \( d-d \), \( d-s \), \( d-p \), \( s-p \). The splitting structure is a sum of the ground state splitting and the excited configuration with taking into account the selection rule for transitions in the quantum numbers. The total number of components can exceed several hundreds. It should be noted that the structure of the \( 5d^4 \) shell is not changed through transitions. This shell has the largest splitting scale but this splitting does not influence on the splitting of lines. The scale of the line splitting is determined by the weak \( s-s \), \( s-d \) interactions. All the transition components are located within the relatively narrow interval determined by these two interactions.

2. The transitions between two excited configurations, for example, \( 5d^46s6p - 5d^46s6d \).

   In this case the \( 5d^4 \) and \( 6s \) shells are not changed through transition. The splitting scale is determined by the outer electron. All the transition components are located within the narrow interval.

3. The transition from an inner shell, for example, \( 5d^46s6p - 5d^36s^26p \).

   This case differs from above mentioned one. The splitting scale of the \( 5d^4 \) and \( 5d^3 \) shells are different. Moreover, there are transitions from an each \( L^5 \) term of the \( 5d^4 \) shell to several deferent \( L_i^5 \) terms of the \( 5d^3 \) shell. Weight of the each transition is proportional to square of the corresponding genealogical coefficient. The specter of the transition consists of several separate groups of lines, each group being similar to transitions of first or second type. Moreover, each group can be located in the different frequency interval and the intensities can significantly differ.

4. The transitions between two groups of equivalent electrons, for example, the transition \( 4f^{14}5d^2 - 4f^{13}5d^3 \) for \( W^{3+} \) ion.

   This type of the transition is most complex. Some components can have the large splitting and appear in the autoionization region in depending on the number of electrons in the shell, ion charge, etc.
In our model we take into account only first three cases and omit fourth one because it is not significant for tungsten. Fourth case can be significant for other heavy elements, for example, uranium. The special algorithm was developed for all the possible quantum states of lower and upper configurations, for calculations of the angle factors, and the genealogical coefficients, which is included into the TOPATOM code.

For tungsten, the spin-orbital splitting should be taken into account in addition to the electrostatic one. Because of large charge of the tungsten nucleus, they are comparable. It should be noted that the spin-orbital splitting has another meaning then for description of the relativistic corrections. In the latter case the single electron interaction between the electron spin and its own orbit is taken into consideration. In this case, the interaction between the total orbital and total spin shell momenta with the further splitting onto $J$ components is taken into account. Here, there are also a lot of different situations. Magnitude and structure of the splitting which depend on whether the interaction within the shell or between different shells are considered. Classification of splitting depends on the splitting scale within each group of electrons. These groups are changed through a transition. Here, we don't list the classification because it similar to the classification of the electrostatic splitting but some significant features are pointed out.

The splitting structure depends essentially on the coupling type in an atom. Tungsten is the element for which the pure type of coupling is not realized. In this case, the intermediate coupling should be taken into consideration with diagonalization of an energy matrix for all the type of transitions being allowed. Such the procedure is used for a precision calculation with several levels and can not be used for total calculation because of the large laborious. In our model ether the $L-L$ or $J-J$ type of coupling is used to calculate the splitting in dependence on which type of coupling dominates. Such a simplification does not make worse the optical properties because the total number of the components and the splitting width remain the same. However, the structure of line components is changed a little. If the distance between the components on frequency is less then the plasma temperature, then the mean absorption and emission coefficients are not changed. After a re-normalization, the specter becomes more realistic. If some experimental energy levels are used together with the experimental ionization potentials, then the experimental values of Slater integrals can be determined and used to calculate the other components of the splitting.

It should be noted that such the re-normalization procedure of the calculated energy levels is essential for neutral atoms and low ionized ions when the HFS and HF methods give the results with a low accuracy. The accuracy of both methods increases with increase of the ionization degree. In this case, the relative scale of electrostatic splitting decreases and the re-normalization procedure is not required. On the other hand, the experimental data [7] exist only for a small
number of ions of the heavy elements, for example, for tungsten there are data only for \( W_1 \) and \( W_2 \) ions.

The above-described procedure is used to correct the spectra of the \( W_1 \) and \( W_2 \) ions. Six terms for the ground configuration \( 5d^46s^2 \) are listed in the table [7] for \( W_1 \) ion. Those are the following terms (in order of energy increase) \( ^5D, ^3P, ^3H, ^3G, ^3F, ^3D \). Really, there are 16 terms for the ground configuration. A known number of the terms is not sufficient to determine all the energy characteristics. In our calculations the ionization potentials and the direct Slater integrals (\( F^0, F^2, F^4 \)) are determined only for the \( d^4 \) shell. For this purpose, the values of energy levels of the \( ^5D, ^3P, ^3D \) terms are used.

The similar procedure is used for the terms of the ground configuration \( 5d^46s \) of \( W_2 \) ion. For other ions, such the procedure is not applicable because of the absence of experimental data.

2.3. Calculation of Ion Concentration and Optical Properties of Tungsten Plasma

The CRE model was used to calculate the ion plasma concentrations and level populations, i.e. the balance equations taking into account the numerous collisional and radiative transitions were used. It is evident that the splitting of energy levels has to be taken into account in the kinetic matrix. The number of kinetic equations corresponding to the number of energy levels increases significantly due to the splitting. As it was mentioned above, there are some difficulties to calculate the rates of the collisional transitions. There is the following way to simplify this problem. The ratio between the radiation and collision rates depends significantly on the magnitude of the transition energy. The rate of spontaneous transition is proportional to \( \Delta E^2 \), where \( \Delta E \) is the transition energy. The rate of collisional transition is proportional to \( \Delta E^{-3/2} \) and \( \Delta E \) is proportional to \( Z^2 \), where \( Z \) is the ion charge. The resonance transition energy is very large for the light elements. Its magnitude can exceed half of the ionization potential. For this reason, the equilibrium close to the coronal one is quickly established with the temperature and average plasma charge increase, when the radiative rates are higher then collisional ones. For the heavy elements the situation is another when the splitting is taken into account. The energy structure is determined by a lot of levels having small value of \( \Delta E \) between them. This structure is still valid for multi-ionized ions. Thus, the collisional transitions dominate upon the radiative ones in the wide temperature and density ranges, and ion concentrations and level populations can be obtained using the Saha-Boltzman assumption.

These arguments are valid if the energy structure consists of the set of closed levels but they are not valid for inner electrons having a large energy scale without the splitting as well as for ions with closed shells. There is no splitting for the closed shells and the specter is similar to hydrogen-like one. For tungsten, there are the following closed shells \( 5p^6, 5s^2, 4f^{14} \), etc.
For tungsten, the calculations of the ion concentrations were performed in the temperature range from 1 up to 20 eV and in a wide density range. Here, we are restricted by the Saha-Boltzmann model.

To calculate the absorption and emission coefficient the procedure similar that for the light elements is used. The total absorption coefficient is the sum of absorption coefficients from all the levels taken with a weight determined by the level population. Some features of calculations that are typical for the heavy elements are listed below. For the light elements the absorption cross section is determined by the oscillator strength, line broadening contour, and frequency. For the heavy elements, it was assumed that the sum of oscillator strengths for the total component is equal to the oscillator strength of the transition between the configurations. Therefore, to determine the oscillator strength of the components it is sufficient to calculate the oscillator strength of transition between the configurations using either the HFS or HF methods. Relative intensities of the components are calculated using the similar characteristics as for calculations of the splitting, that is the Slater integrals, genealogical coefficients, $3nj$-symbols, etc. The expressions are not presented here due to its inconvenience.

It is also assumed that all the line components have the similar broadening and the contours are the same. In this case, it is also sufficient to calculate parameters of broadening and to normalize the contour for the non-splitting transition between the configurations. The relative distance between the components is determined by the splitting scale of the lower and upper configurations. Thus, due to the splitting a single transition between the configurations is splitted into a lot of components having the different intensities.

All of the above mentioned features refer to the continuum. The absorption in continuum (except the bremsstrahlung) is determined by the sum of processes from the levels. The absorption from each level is determined by the photo-ionization cross section, which can be calculated using either the HFS or HF method. The splitting of the levels leads to the splitting of the photo-ionization thresholds. The relative weight of each threshold is proportional to the probability of its realization. Here, the following assumption is made. The photo-ionization cross sections of the components are equal and correspond to the photo-ionization cross section from the configuration.

### 2.4. Results and Discussion

The above mentioned method of calculations was realized as a computer code which was used to calculate the ion concentrations of a tungsten plasma in the wide temperature and density ranges: temperature range from 0.5 eV up to 20 eV, density range from $10^{16}$ up to $10^{19}$ cm$^{-3}$ which cover the tokamak disruption problem modeling. Validity limits of the used model are restricted by the same ranges. It should be noted that an investigation of the heavy element spectra is
very complex problem. At present, there are not fully developed conceptions to solve this problem. Therefore, this report should be treated as the first step.

As it was assumed, the structure of absorption coefficients of the tungsten plasma is very complex. In Figs. 1-3, one can see the absorption coefficients of the tungsten plasma for several temperatures and densities. For the low frequencies \((E<T)\) the absorption is determined by the bremsstrahlung and is a smooth function of the frequency. The main part of the line transitions is non-uniformly located within the \(T<E<10T\) range with line intensities having a non-regular character. Some parts of spectra include a lot of lines from a quasi-continuum. For frequencies higher then \(10T\) the absorption coefficients are determined by the photo-absorption from the inner shells and are smooth functions of the frequency.

As it has been mentioned, above all the calculations were performed using the Saha-Boltzman assumption. In this case, the emission coefficients \(\beta\) are associated with absorption ones \(\kappa\) by means of the following expression \(\beta=\kappa U_\nu\), where \(U_\nu\) is the Planck function. This expression is valid for frequencies up to \(10T\), i.e. for the ground and excited levels. However, it can not be used for the inner shells. The real emission coefficients have to be less then calculated ones using this expression. However, a maximum of the Planck function is located about \(3T\). Therefore, the contribution of frequency range \(E>10T\) into the total emission is not so large and an error in emission coefficients will not leads to the large error in the total plasma emission.

It is interesting to compare our result with others. Comparisons with data [8] are presented in Figs. 3-5. In work [8] authors use the method close to that described in item 2, i.e. the statistical method of the splitting was used. The resulting specter consists of the very broaden lines (transitions between configurations with the width being equal to the splitting one), bremsstrahlung, photo-continuum. One can see that there is a good agreement in the bremsstrahlung, therefore ion concentrations are similar. There is sufficient agreement in the lines. The forms and amplitudes of the lines are different due to the different approach for taking into account of the line splitting. In our calculations, all the components with real width of the splitting were taken into account. Due to this reason, the lines have large amplitude in the centers and a quick decrease in the wings. Opposite, in the work [8], the amplitudes of lines are not so large and there is not detailed structure of lines (see Figs. 4-5). To compare both results more carefully we performed averaging of our results over the spectral groups having the width coinciding with the splitting width. In result, we have obtained the spectra reminding that from the work [8] (see Fig. 6). The complete agreement can not be achieved because the averaging procedure of the detailed specter is not adequate to the procedure of statistic description of the splitting.

A comparison of the absorption coefficients obtained using the common CRE model without the splitting with the results with taking into account the splitting is
presented in Fig. 7. There is a large difference in absorption coefficients that can lead to a large divergence in results of the radiation transfer calculations.

Absorption and emission coefficients are usually used for calculations of radiation transfer in the plasma. The radiation transport in the lines is a complex problem. For the adequate calculations of the radiation transport within a line the rather large number of spectral points have to be used. The detailed description of a line is not possible if there are a lot of lines in a specter. In this case, either the Planck or Rosseland group coefficients have to be used in the radiation transfer calculations. As it has been mentioned above, only the detailed description of the splitting allows obtaining the mean Rosseland coefficients with a good accuracy.

Either absorption or emission line spectra are sometimes used to identify the individual lines or for the plasma diagnostics. However, calculated absorption tungsten spectra can not be used for these purposes due to its complexity and there is not sufficient accuracy to determine the individual line components.

![Absorption coefficient vs photon energy](image)

Fig. 1 Tungsten plasma T=1 eV, N=10^{17}\text{cm}^{-3}
Fig. 2  Tungsten plasma  $T=1$ eV, $N=10^{17}$ cm$^{-3}$

Fig. 3  Tungsten plasma  $T=10$ eV, $N=10^{19}$ cm$^{-3}$
Fig. 4  Tungsten plasma  $T=10$ eV, $N=10^{17}$ cm$^3$

Fig. 5  Tungsten plasma  $T=10$ eV, $N=10^{17}$ cm$^3$
Fig. 6 Tungsten plasma $T=10$ eV, $N=10^{18}$ cm$^{-3}$

Fig. 7 Tungsten plasma $T=1$ eV, $N=10^{17}$ cm$^{-3}$
3. Theory of Electrostatic and Spin-Orbital Splitting

The mathematical technique of atomic physics and its terminology is very complex. We shall briefly remind some basic concepts to facilitate the understanding of further exposition. The independent variables in the Schrödinger equation of an atom can be divided. Thus, the radial wave functions can be found from the HF or HFS equations [9,10]. The angular functions are found separately with use of the mathematical technique of summation of the electron moments. It should be noted that the orbital and spin moment summation in the quantum mechanics is not commutative operation, i.e. the result of summation depends on the sequence of performed operations. In principle, there are \((2^n)!\) ways to carry out the summation for \(n\) electrons with an orbital and spin moment. However, there are the most probable ways of a moment summation. First, the moments with the greatest energy are summed, and then step-by-step the moments with smaller energy is added in the order of their decrease. Such a method of moment summation was named as the principle of genealogical scheme. Depending on the ratio of energies of two electrons the different schemes are realized: first, the summation with respect to orbital moments of all the electrons is performed, second, all the spin moments is separately summed, and finally, the total orbital moment is added to the total spin one. It is the \(LS\)-coupling. The summation of the orbital electron moment with the intrinsic spin and then the consecutive addition of these moments are the \(JJ\)-coupling. The different intermediate combinations are also possible. In the case of low-\(Z\) elements (up to \(Z \approx 30\)) the \(LS\)-coupling is valid with a good accuracy. In the case \(Z \approx 90\), the \(JJ\)-coupling is valid with a greater accuracy. For the group of equivalent electrons in the \(nl^q\) shell, all the electrons have an identical energy. In this case, the principle of genealogical scheme is a poor approximation. The term with quantum numbers \(LS\) can be obtained in several ways. The \(LS\) term is obtained by addition of one electron \(ls\) to the frame with quantum numbers \(L_0S_0\): \(L_0S_0 + ls = LS\). If the \(l\) value is large, then a number of variants of the \(L_0S_0\) numbers is also large. The summation scheme of equivalent electrons is carried out in the approach of genealogical scheme. The calculation manners of genealogical coefficients and the classification of groups of the equivalent electrons are named the Racah technique [11-13]. The transition coefficients from one type of coupling to other
one are determined by the values, which are named $3nj$-symbols. The $3j$, $6j$, $9j$ and $12j$-symbols are used more often. The symbol number denotes the number of moments and intermediate summands. Below we use the approximation of the $LS$-coupling and genealogical scheme. The deviation from this approximation will be especially discussed.

In the calculations of the spectroscopic characteristics, the HFS method is used. The HFS method gives a possibility to calculate the energy levels of the $nl^q$ configurations, where $n$ is the principle quantum number, $l$ is the orbital quantum number, $q$ is the number of equivalent electrons in the shell. In the case of filled shells, the total orbital moment $L$ and total spin moment $S$ are equal to zero. In the case of unfilled shells, the variety of the $L,S$ numbers is possible. The energy $E(n,l,q,L,S)$ of each term depends on these numbers. The additional quantum number $v$ is used to describe the $d$-shells. This number is necessary to differ some terms with the same $LS$. The number $v$ defines the minimum value $q$ for which the term with given value $L,S$ is occurred for the first time. The additional quantum numbers $U$ and $W$ are introduced to describe the $f$-shells [13]. The sense of these numbers has not the simple explanation as $v$. The exact value of the energy level is determined by all the quantum numbers $n,l,q,L,S,v,U,W$. It is necessary to use the multi-configuration Hartree-Fock (MHF) method for each set of quantum numbers to calculate the characteristics of energy levels. In the case of the high- $Z$ elements, the spin-orbital splitting becomes comparable with the electrostatic one. In this case, it is necessary additionally to use the total moment $J$. For the $d^5$-shell a number of possible terms is $N_1=16$. For the $f^7$-shell, this number reaches $N_2=119$ (without taking into account the splitting in $J$). The interaction of two unfilled shells produces a number of terms $N_1*N_2$. Thus, the use of the MHF method is associated with a very large amount of work. The opportunity to use the MHF method with reference to the $d^9$ and $f^9$-shells is still poorly investigated.

In the present work, the method of the perturbation theory was used. The following assumption was made. All the terms of the $nl^q$-shell have the same radial wave functions. The radial wave functions are calculated using the HFS-method. The angular wave functions are different that for different terms. In this case, the interaction energy inside this shell is determined by the formula [10,13]
Here, $\alpha$ is the set of quantum numbers $v,U,W$. $F_k$ is the Slater integral determined by the formula

$$E(n,l,q,L,S,\alpha) = \sum_k F_k(nl,\alpha_l) f_k(l,q,L,S,\alpha).$$

$$F_k(n_l, n_{l_2}) = \int P_{\alpha l l}(r) P_{\alpha 2 l 2}(r_i) \frac{r_{\alpha}^k}{r_{\alpha+1}^k} P_{\alpha l l}(r_i) P_{\alpha 2 l 2}(r) dr dr_i.$$ 

Here, $P_{\alpha l l}$ and $P_{\alpha 2 l 2}$ are the HFS radial wave functions for the $n_1l_1$ and $n_2l_2$ quantum states. The $r_{\alpha}$ and $r_{\alpha+1}$ values are the smaller $r$ and greater $r_i$ radiuses of electrons, respectively. Index $k$ determines the multiplicity $0 \leq k \leq 2l_{\text{min}}$. The value $f_k(l,q,L,S,\alpha)$ is the angular multiplier, which is determined by the methods of the Racah technique. Below the method to calculate these values is described in more details. The interaction between the shells is described by [13]

$$E(n_1l_1, n_2l_2, \alpha_1; n_1l_2, n_2l_2, \alpha_2) = \sum_k F_k(n_1l_1, n_2l_2) a_k(n_1l_1, n_2l_2, \alpha_1; n_1l_2, n_2l_2, \alpha_2) + \sum_k G_k(n_1l_1, n_2l_2) b(n_1l_1, n_2l_2, \alpha_1; n_1l_2, n_2l_2, \alpha_2).$$

Except the Slater integral $F_k$ there is the exchange integral $G_k$

$$G_k(n_1l_1; n_2l_2) = \int P_{\alpha l l}(r) P_{\alpha 2 l 2}(r_i) \frac{r_{\alpha}^k}{r_{\alpha+1}^k} P_{\alpha l l}(r) P_{\alpha 2 l 2}(r) dr dr_i,$$

where $a_k$ and $b_k$ are the angular functions of interaction between the shells.

Many physical values are calculated using the HFS radial wave functions. It is the $F_k$ and $G_k$ integrals, oscillator strengths for transitions between the $n_1l_1-n_2l_2$ configurations, the photoionization cross-section. These characteristics are calculated in the first part of a problem. Then, these characteristics are stored in the special bank of spectroscopic data for all the type ions of the plasma. The $f_k$, $a_k$ and $b_k$ values depend on all the set of quantum numbers. The calculation of these values is the most difficult problem. These values are calculated in the second part of problem together with of the absorption and emission spectra.

3.1. Calculation Methods for $f_k, a_k, b_k$ Characteristics
The $f_k, a_k, b_k$ functions are expressed by complex algebraic formulas. These formulas contain some standard functions of the theory of complex spectra. Those are genealogical coefficients, reduced matrix elements of the spherical function, submatrix elements of the $U$ and $V$ tensor operators, $3nj$-symbols. Let us describe these functions

- the genealogical coefficient $G_{L1S2}^{L2S2r2}$ determines the realization probability of the term with the $L_2S_2$ quantum numbers when the electron is removed from the shell with the $L_1S_1$ quantum numbers. The genealogical coefficients are found as a result of solution of the system of algebraic equations. For the $p^9$, $d^9$, $f^2 - f^4$ and $f^{10} - f^{14}$-shells the genealogical coefficients are contained in the tables and are used to calculate the term splittings. The matrix elements determined by means of integrals from different wave functions should also depend on the magnetic quantum numbers $m$. The $m$ number determines a value of moment projection on the given axis. For matrix elements of an atom the division of variables with the $l$ and $m$ quantum numbers (the theorem by Eccart-Wigner) is possible. The matrix elements which don't contain the dependence on $m$ is referred below as the reduced matrix elements [13].

- the reduced matrix elements of the spherical $(l\|C^k\|_l)$ function were calculated for a large number of orbital numbers $l$ and the multiplicity $k$, and are contained in the tables.

- the $3nj$ symbols are calculated by means of algebraic methods. The $3j$, $6j$ and $9j$ symbols are usually used. In the given work, the calculation method of all these values was realized.

- the submatrix elements of the $(l^qLS_\alpha\|U^k\|l^qL_\alpha)$ and $(l^qLS_\alpha\|V^{1k}\|l^qL_\alpha)$ tensor operators determine the interaction between the different terms of one configuration. These values are expressed by complex algebraic formulas. These formulas include the genealogical coefficients, the $3nj$-symbols, and the reduced matrix elements of the spherical function. In the given work, the calculation of these values was also realized.

Taking into account the above discussion the expression for the interaction energy inside the shell can be presented by the following formula [13]

$$f_k = \frac{q}{2} \left( \frac{l\|C^k\|_l}{2l+1} \right)^2 \left\{ \frac{1}{q} \frac{2l+1}{2L+1} \sum_{l=1}^{L} \left( l^qLS_\alpha\|U^k\|l^qL_\alpha \right)^2 - 1 \right\}.$$
The $a_k$ and $b_k$ functions have the similar structure but they are very complex. All these functions are evaluated during the calculation process of the splitting value. The interaction energy $f_k$ depends on all the set of quantum numbers and the multiplicity $k$. Thus, the number of the $f_k, a_k, b_k$ characteristics is determined by a number of sets of the quantum numbers. The relative value of splitting is determined by the difference of these values. The form of $f_k, a_k, b_k$ functions depends on the coupling type between the electrons. All the presented formulas are written for the $LS$-coupling. The similar formulas can be written in the extreme case of $JJ$-coupling. These formulas are more complex for an intermediate type of coupling. In the given work, the splitting for the intermediate type of coupling was studied approximately. We have used a linear combination of two extreme types of $LS$- and $JJ$-coupling.

### 3.2. Calculation of Spin-Orbital Splitting

The value of spin-orbital splitting for the high-Z elements is comparable to the electrostatic one. For the atom with one extra electron outside the filled shell, the value of spin-orbital splitting is determined by the following formula

$$\xi_{nl} = \int \frac{1}{r} \frac{dU}{dr} P_{nl}^2(r) dr,$$

where $U$ is the potential inside the atom, $P_{nl}$ are the radial wave functions. In the given work, the HFS wave functions are used. The $\xi_{nl}$ values are calculated for all the states and are contained in the bank of spectroscopic data. In the case of $LS$-coupling for the unfilled shells with the equivalent electrons the splitting is determined by the Lande rule [10]

$$\Delta E_j = \frac{1}{2} A(L, S, \alpha) \{ J(J+1) - L(L+1) - S(S+1) \}.$$

The Lande constant $A(L, S, \alpha)$ for one unfilled shell is determined as follows

$$A(l^q, L, S, \alpha) = \xi_{nl} \sqrt{\frac{l(l+1)(2l+1)}{S(S+1)(2S+1)L(L+1)(2L+1)}} (l^q LS \alpha \parallel l^q LS \alpha)$$

The interaction of two shells is determined by the complex algebraic formula containing the $A$ values for different shells. In the case of $JJ$-coupling the value of splitting is determined by the formula

$$\Delta E_j = \frac{1}{2} \xi_{nl} \left\{ j(j+1) - l(l+1) - \frac{3}{4} \right\},$$

$$$$
where \( j = l \pm 1/2 \). In the case of intermediate coupling, it is also possible to use a linear combination of two above formulas.

### 3.3. Numerical Calculation of Splitting

In the previous items, the methods for calculation of the electrostatic and spin-orbital splitting were presented. The splitting of spectral line is determined by the splitting of the lower and upper levels. The described above technique was realized for the \( p^q -, d^q -\) shells, \( f^2 - f^4 -\) shells and \( f^{10} - f^{14} -\) shells. The realization of this technique for the \( f^5 - f^9 -\) shells is more difficult. It determined by the several reasons. The main difficulty is the calculation of the genealogical coefficients for these shells. The spectra of the \( f^5 - f^9 -\) shells are much more complex than the spectra of the \( f^4 - f^{10} -\) shells. The spectra of the \( f^4 - f^{10} -\) shells contain a very large number of the spectral components. The intensity distribution of the components is close to the normal law. In this case, it is possible to assume that the spectra of the \( f^5 - f^9 -\) shells will be also distributed in accordance with the normal law. In this case, it is necessary to determine the interval between the minimal and maximal components of the splitting, the number of components, and to distribute these components in accordance with the normal law. This procedure was realized for the \( f^5 - f^9 -\) shells.

The splitting calculation is performed simultaneously with the calculation of the absorption and emission spectra. The calculation of the \( a_k \) and \( b_k \) characteristics is the most difficult. It should be noted that the existence probability of two unfilled shells in a multi-charge ion is very low if there is more than one electron in both shells. For the neutral tungsten atom the \( 5d^4 6s^2, 5d^4 6p^2 \) and \( 5d^4 6s6p \) states are only realized. For the tungsten ions, the \( n^l n_1 l_1 \) states are usually realized. In the second unfilled shell, there is only one electron. In this case, the expressions for the \( a_k \) and \( b_k \) coefficients are significantly simplified. In the given work for all the complex shells the preliminary calculation of the \( a_k \) and \( b_k \) characteristics is performed and they are stored in a databank. In a case of one extra electron outside the shell, these calculations are performed simultaneously with the calculation of the absorption spectra. The splitting of the energy levels are taken into account at calculation of the wavelength of a spectral line and it relative intensity. The splitting is taken into account at determination of the photoabsorption threshold and level population.

### 4. Calculation of Relative Line Intensities with Taking
In the previous sections, the values of the splitting energy were calculated. The total intensity of transition between the configurations is also distributed between the spectral components. The value of line intensity is determined by the oscillator strength of the transition between $nl$ and $n_l l_j$ states [10]

$$f(nl, n_l l_j) = \frac{2m\Delta E}{3h} \frac{l_{\text{max}}}{2l+1} R^2,$$

$$R = \int P_{nl}(r)P_{n_l l_j}(r) dr.$$

Here, $\Delta E$ is the transition energy, $m$ is the electron mass, $h$ is the Planck constant, $l_{\text{max}}$ is the maximum of two numbers $l, l_j$. The radial matrix element $R$ of the transition is a function of the integral from the $P_{nl}$ and $P_{n_l l_j}$ radial wave functions. In this case, the HFS wave functions are used. The given value of the oscillator strength is a sum of all the components. To calculate the specified component it is necessary to multiply the oscillator strength $f$ by the factor [10]

$$(G_{L0S0}^{LS})^2 \frac{2L_0 + 1}{2L + 1} Q(SLJ; SL_l l_j) Q(L_0 L; L_0 l_j l_j).$$

Here, $G_{L0S0}^{LS}$ is the genealogical coefficient of the shell with the $l, L, S, J$ quantum numbers from which the transition is occurred. After the electron transition, the residual shell has the $L_0, S_0$ quantum numbers. In the final state, the system "residual shell+exited electron" has the $l_j, L_j, S, J_j$ quantum numbers. The $Q$ functions are expressed by means of the $6j$-symbols [10]

$$Q(SLJ; SL_l l_j) = \left( \frac{2J + 1}{2S + 1} \right)^2 \frac{(2J + 1)(2J_j + 1)}{2S + 1} \left\{ \frac{LJS}{J_l L_i l_j} \right\}^2.$$

Here, $\left\{ \frac{LJS}{J_l L_i l_j} \right\}$ is the $6j$-symbol. The first $Q$-factor describes the spin-orbital splitting of the intensity components. The second $Q$-factor describes the electrostatic splitting of the intensity components. For the intensities of transitions, the selection rules of dipole radiation are used: $\Delta l = \pm 1$, $\Delta L = 0, \pm 1$, $\Delta J = 0, \pm 1$, $\Delta S = 0$. 

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5. Calculation of Charge States and Populations of Levels

To calculate the charge states and the population of levels the collision-radiative approximation is used. In this case, it is necessary to solve the system of linear algebraic equations with the number of equations equal to the number of levels. With taking into account the electrostatic and spin-orbital splitting, each $nl$ state can have several tens or hundreds of levels. The total number of levels in an ion can reach several thousands. The solution of such the system of equations is a complex problem.

The radiative dipole transitions between the components of one $nl$ configuration are forbidden by the selection rules ($\Delta l = 0$) but the collision transitions are allowed. Thus, if to neglect by the multipole radiation, then the Boltzman equilibrium is reached between the splitted components of one $nl$ configuration. In this approximation, it is possible to calculate the charge state and the relative populations of levels between the $nl$ configurations. The Boltzman equilibrium is reached between the specified configurations. In this case, the common collisional-radiative model is used. However, there is the essential difference. The transition rates between the $nl$ configurations are the integrated values consisting of a large number of the transition components. If two configurations have the $N_1$ and $N_2$ components of levels, then the total number of components of the collisional transitions between the configurations will be about $N_1 \times N_2$. Each ion has about 200-400 $nl - n_l l_i$ transitions. The problem is solved by means of the method of iterations and such a method requires an enormous amount of computer time. It is necessary to enter further simplifications.

Let us consider the most probable case. There is one extra electron outside the shell. Let it is the $4f^45p$ configuration. The $4f^4$-shell has 47 terms with the different values of the $LS\alpha$ quantum numbers. At addition of the $5p$-electron, each of these terms forms the new system of splittings (for the majority of terms - 6 levels). Hence, the total number of levels in this configuration will be more than 250. Similarly, it is possible to determine the number of levels for the $4f^45d$ configuration. It is about 450. The total number of components of the $4f^45p - 4f^45d$ collisional transitions is about $10^5$. For the accurate account of these transitions, it is necessary to take into account all $10^5$ components.

It should be noted that the splitting of the $4f^45p$ configuration has two different scales. The splitting scale of the $4f^4$ shell can be large and comparable with the value of ionization potential. The scale in many respects depends on the
effective ion charge. The splitting associated with the interaction of the $LS\alpha$ term with the $5p$ electron has the considerably smaller scale. At the $4f^4 5p - 4f^4 5d$ transition, the $LS\alpha$ quantum numbers of the $4f^4$-shell are not changed. The lengths of waves of all $10^5$ transitions will differ by an insignificant value. In this case, it is sufficiently to find the average energy of transition and to choose the characteristic transition rate for all the components.

For the $4f^4 - 4f^3 5d$ or $4f^4 5p - 4f^3 5p 5d$ transitions the situation is much more difficult. In this case, the scale of the line splitting is directly determined by the splitting scale of the $4f^4$-shell. In this case, it is necessary in details to take into account all the components.

In the given work, the following method to solve above a problem is suggested. Let us consider the typical transition rate of the collisional excitation, which is described by the Van Regemorter formula [14]

$$\langle v\sigma_{12}\rangle = 3.2 \times 10^{-7} f_{12} \left( \frac{Ry}{\Delta E} \right)^{\frac{1}{2}} \left( \frac{\Delta E}{T} \right)^{\frac{1}{2}} \exp\left( -\frac{\Delta E}{T} \right) \sigma(\Delta E/\tau).$$

The $\langle v\sigma_{12}\rangle$ transition rate between the states 1-2 is proportional to the corresponding oscillator strength $f_{12}$, and depends also on the ratio between the transition energy $\Delta E$ and the temperature $T$. Especially the strong dependence on the ratio $\Delta E/T$ is contained in the exponential function ($\sigma$ is a slowly varied function). It is obvious that at the large scale of the splitting the $\langle v\sigma_{12}(\Delta E_i)\rangle$ value is significantly differed from the $\langle v\sigma_{12}(\Delta E)\rangle$ value. The first value is the average rate of the collisional transition. The second one is the rate as a function of the average energy of transition. We shall denote $\delta E$ as the interval between the minimal and maximal components of the splitting. For each set of the $\Delta E$ and $\delta E$ values it is possible to create the table of the corrections between the $\langle v\sigma_{12}(\Delta E_i)\rangle$ and $\langle v\sigma_{12}(\Delta E)\rangle$ values for a wide range of $\Delta E/T$ ratios. In this case, it is possible to use the integrated $\langle v\sigma_{12}(\Delta E)\rangle$ ratios of transitions, for example, the $4f^4 - 4f^3 5d$ configurations, with the corresponding correction. In the given work, the calculations were carried out with use of the correction function described above. The example of the correction function for the collisional discrete transitions was presented above. The similar functions were created for the other ratios: collisional ionization, photorecombination, and spontaneous transitions.
These tables were previously tabulated and are stored in the databank of spectroscopic information. Thus, the calculation problem of the ionization balance and the populations of levels with taking the electrostatic and spin-orbital splitting into account is possible to reduce to the collisional-radiative model used for the low-$Z$ elements.

6. Calculation of Optical Spectra

The splitting procedure is realized for photoabsorption thresholds and spectral lines. In the first case, one threshold is decayed into the set of fine ones and the total threshold becomes non-sharp. The weight is assigned to each photoabsorption component, which is proportional to the level populations. The exited configurations have such a structure of the photoabsorption. The structure is more complex at photoionization from the shell with the equivalent electrons. For example, in the case of the $f^4$ shell the $L,S,\alpha$ terms have 20-30 possible genealogical states. Own threshold corresponds to each genealogical state. These thresholds will have a fine structure corresponding to the interaction of the $f^4$ shell with the exited electrons.

The splitting calculation in lines is more complex and requires excessive computer time. It is explained by a fact that a number of the spectral lines is significantly greater then a number of the photoabsorption thresholds. In addition, it is necessary to calculate the line contour for each component. In the given work, the assumption is taken that the line width is the same for the total set of components of the $nl - n_l l_1$ transition. Such an assumption is quite reasonable. The line broadening is mainly determined by the broadening of the upper $n_l l_1$ level having the small scale of splitting.

Thus, the calculation of spectral line contour is carried out for the transition between the $nl - n_l l_1$ configurations. Then this contour is used for the transition component with taking the populations of components of levels and the relative intensity of components of transitions into account. The total spectrum is very complex. We shall consider several typical situations, which can be realized in the tungsten plasma.

- Low-temperature plasma with the temperature in a few eV. In this case, the degree of ionization is insignificant and the $5d^2 6s^2$, $5d^4 6s$, $5d^4$, $5d^3$-shells are available in the plasma. The splitting structure of the $5d^4$-shell has a large scale. The interval between extreme terms reaches half of the ionization potential. The linear spectrum will be presented by a large number of
components and the components are within a large frequency interval. Each component can have the fine interaction structure of the $5d^4$-shell with an exited electron. The interval between the neighboring components is usually larger than the line width, and the spectrum consists of a large number of individual lines.

- Temperature in the plasma is about 20 eV. The $5d$-shell is completely ionized and the ions with the $5p$-shell are present in the plasma. The spectrum is significantly simplified as the number of states into the $p$-shell is much less than into the $d$-shell. The spectrum consisting from separate lines in many respects reminds the spectrum of low-$Z$ elements. The most simple spectrum is for the $5s^2$-, $5s^-$, and $4f^{14}$-shells, and it reminds the He-like or H-like one.

- Temperature is about 50 eV. The $f$-shell is ionized and the spectrum is the most complex. The number of spectral lines is significantly greater than in the case of the $d$-shell. The $f$-shell has very a large scale of splitting but in the case of tungsten the $f$-shell is realized at ionization degrees about $z \approx 20$.

For this reason, the interval between the extreme terms makes 15-20% from the ionization potential and all the components of lines are found in rather narrow intervals of frequencies. In this case, the situation can be realized when the interval between the components of lines is less than the line width, and the spectrum is transformed from linear into the quasi-continuum one of complex form.

We shall note one detail, characteristic only for the $f$-electrons. For the low-$Z$ elements, the ground states are the most probable. Therefore, the spectrum includes mainly the resonant series with the small additives of the exited transitions. Let us consider now the $4f^{12}$-configuration. The statistical weight of this configuration is equal to 91. At excitation of one electron the $4f^{11}5s$ or $4f^{11}5p$ configuration will be formed. The statistical weight of the $4f^{11}$-configuration is equal to 364. The statistical weight of the $4f^{11}5s$ and $4f^{11}5p$ configurations will make 728 and 2184, respectively. The excitation energy of the $5s$ and $5p$ electrons is very low. Therefore, the $4f^{11}5s$ and $4f^{11}5p$ configurations will have larger population than the $4f^{12}$ ground state. For this reason, in the spectrum a large number of strong lines from exited states will be observed. If the $f$-shell has seven or less electrons, then this effect is
disappeared. In this case, at excitation of one electron the statistical weight of the frame is decreased.

To demonstrate the described effects the calculation of the charge state and the populations of levels of the tungsten plasma was performed at the temperature in 50 eV. At calculation of the absorption spectra only one ion W\(^{18}\) having the \(f^{11}\)-shell was taken into account. For a comparison, the calculations of the spectrum of this ion without the account of splitting in CRE and LTE approximations were also carried out. For the important transitions the identification is presented in Figs. 25, 26. A comparison of three different variants shows large distinctions in the results. The account of splitting results to the strong qualitative and quantitative changes. The optical thickness is significantly decreased in the center of absorption but the width of the absorption interval is considerably increased. These distinctions will change the character of the radiation transfer by an essential manner. One can assume the models of radiation transfer should be different in the different types of spectra. Thus, at the temperature about 20 eV the spectrum reminds that of the low-\(Z\) elements, and consequently the transfer models should be adequate. In the situation at the temperature about 50 eV when the complex linear spectrum forms the quasi-continuous one, it is possible to use the transfer models of continuous spectrum. The situation at the temperature about a few of eV is the most complex when the spectrum is a large number of individual lines.

In the given calculations the small-scale group method is used instead the spectral one. In this case, the value \(\int_{\omega_0}^{\omega_0+\Delta\omega}\phi(\omega)d\omega\) is calculated, where \(\phi(\omega)\) is the line contour and \(\Delta\omega\) is the interval of averaging. If there are a lot of lines, then many lines can be found in the \(\Delta\omega\) interval. In this case, the spectrum is strongly averaged. The number of individual-resolved lines becomes larger at a decrease of the averaging interval. Thus, the spectra have the properties of fractal objects. It is shown in Fig. 27. The spectra of the \(f^{11}\)-shell with the degree of resolution of 1000, 2000, and 5000 points per the frequency order are presented. In Fig. 27, one can see that a number of "found out" lines is considerably greater for the case of 5000 points. The last detail shows that any manners of averaging for such the spectra will give serious errors in the radiation transfer and it is necessary to develop the statistical methods of radiation transfer for such the spectra.

**7. Optical Spectra of Tungsten**
All listed above moments were taken into account to calculate the tungsten spectra. The calculation was carried out for a wide range of temperatures, densities, and energies of photons. The density range is $10^{15}-10^{20}$ cm$^{-3}$, with the step of half-order. The temperature is changed from 0.5 up to 200 eV with the step of 1.259 (10 points per order). The frequency is changed in the range 0.1-2000 eV within an uniform logarithmic scale with 1000 points per order. The absorption and emission coefficients are calculated in the traditional form as two absorption coefficients measured in cm$^{-1}$. Below in figures several characteristic spectra are presented for a various set of temperatures and densities. Absorption coefficients for the tungsten plasma at the temperature 50 eV and density $10^{18}$, $10^{16}$ cm$^{-3}$ are shown in Figs. 8-27.
Fig. 9 Tungsten plasma $T=50 \text{ eV}$, $N=10^{18} \text{ cm}^{-3}$

Fig. 10 Tungsten plasma $T=50 \text{ eV}$, $N=10^{18} \text{ cm}^{-3}$
Fig. 11  Tungsten plasma  $T=50$ eV, $N=10^{18}$ cm$^{-3}$

Fig. 12  Tungsten plasma  $T=50$ eV, $N=10^{18}$ cm$^{-3}$
Fig. 13  Tungsten plasma  $T=50$ eV, $N=10^{18}$ cm$^{-3}$

Fig. 14  Tungsten plasma  $T=50$ eV, $N=10^{18}$ cm$^{-3}$
Fig. 15 Tungsten plasma $T=50$ eV, $N=10^{18}$ cm$^{-3}$

Fig. 16 Tungsten plasma $T=50$ eV, $N=10^{18}$ cm$^{-3}$ (only shell 4f$^{11}$, W18)
Fig. 17 Tungsten plasma $T=50$ eV, $N=10^{16}$ cm$^{-3}$
(only shell 4f$^{11}$, W18)

Fig. 18 Tungsten plasma $T=50$ eV, $N=10^{16}$ cm$^{-3}$
(only shell 4f$^{11}$, W18)
Fig. 19  Tungsten plasma  $T=50$ eV, $N=10^{16}$ cm$^{-3}$  
(only shell 4$f^{11}$, W18)

Fig. 20  Tungsten plasma  $T=50$ eV, $N=10^{16}$ cm$^{-3}$  
(only shell 4$f^{11}$, W18)
Fig. 21  Tungsten plasma  $T=50$ eV, $N=10^{16} \text{cm}^{-3}$  
(only shell $4f^{11}$, W18)

Fig. 22  Tungsten plasma  $T=50$ eV, $N=10^{16} \text{cm}^{-3}$  
(only shell $4f^{11}$, W18)
Fig. 23  Tungsten plasma  $T=50$ eV, $N=10^{16}$ cm$^{-3}$
(only shell $4f^{11}$, W18)

Fig. 24  Tungsten plasma  $T=50$ eV, $N=10^{16}$ cm$^{-3}$
(only shell $4f^{11}$, W18)
Identification of lines (only shell 4f$^{11}$, W18)

Fig. 25 Tungsten plasma $T=50$ eV, $N=10^{16}$ cm$^{-3}$
Identification of lines (only shell 4f$^{11}$, W18)

Fig. 26 Tungsten plasma $T=50$ eV, $N=10^{16}$ cm$^{-3}$
Identification of lines (only shell 4f$^{11}$, W18)
8. Lebesgue Method of Radiation Transfer in Plasma of high-Z Elements

Absorption and emission coefficients of the high-Z element plasma consist mainly of a lot of the splitted and overlapped lines. To resolve a line in details it is necessary to use several frequency intervals. Thus, the total number of frequency groups to be used in the transfer equations can reach a few of thousands for the low-Z elements and a few of tens - hundreds thousands for the high-Z elements.

Such a drastic rise of a frequency group number (for high-Z elements) can be explained by the following. Let $\Delta\omega_m$ is the width of m-th spectral group, $\Delta\omega$ is the character distance between nearest components of the line splitting, $\Delta\omega_l$ is the typical width of the line (the maximal value from either the Lorentz or Doppler width is assumed). In dependence of the temperature and density, the following situations are realized, for example, in the tungsten plasma.

$\diamond \Delta\omega_m \gg \Delta\omega_0$. It is the typical situation for the $p$ and $s$ shells at rather large densities. In this case, several spectral groups can describe each spectral line as for the low-Z elements.
\[ \Delta \omega \ll \Delta \omega_m \]. In this case, several lines are contained within the spectral group. Therefore, the spectral lines can not be resolved as the single one and the width of spectral group \( \Delta \omega_m \) determines only the accuracy of specter resolution. The number of resolved lines increases with decreasing the width of spectral groups as one can see in Figs. 28, 29, where the typical absorption coefficients are plotted with the resolution of 1000 and 5000 points per the frequency order. Thus, the absorption and emission coefficients have the fractal character. This situation is typical for the unfilled \( d \)-shells. In particular, this situation is realized for tungsten ions at rather low temperatures (0.5-10 eV) where the main ions have the unfilled \( 5d \)-shell.

\[ \Delta \omega \ll \Delta \omega_m, \Delta \omega \ll \Delta \omega_f \]. In this case, the distance between the line components is less then either the group width and the width of lines. It is the case of strongly overlapping lines. A large set of these lines produces some quasi-contiuum, strongly differing from the typical spectral lines. In this case, the decreasing width of spectral groups will not lead to any change of the shape of absorption coefficients and the absorption and emission coefficients will have no the fractal structure. It is a typical situation for the unfilled \( f \)-shells. In particular, this situation is realized for tungsten ions at temperatures about 30-100 eV where the main ions have the unfilled \( 4f \)-shell.

Preliminary estimations shown that the frequency scale with 5000 points per the order is the minimal value when the problem of radiation transfer in the high-Z element plasma can be solved with a rather good accuracy.

Also the number of the base temperature points in the tables of optical properties have to be increased at least to 20 points per order for the high-Z element plasma. In this case, a simple interpolation procedure remains correct. It is due to the fact that ion concentrations are insignificantly changed at such a temperature step (see Figs. 30, 31). For example, an increase of the plasma temperature by 25% (in the temperature range 30-100 eV) leads to the entire change of the ion balance in the plasma, and the absorption coefficients in two neighboring temperature points does not correlate one with another.

Using of the above detailed absorption coefficients in two-dimensional R-MHD calculations would require extremely excessive computational time and memory. Therefore, it is necessary to perform the frequency averaging of optical coefficients.
This is usually done by means of the Rosseland and Planck averaging of the $\beta_m$ and $\kappa_m$ coefficients. The Planck averaging is performed according to

$$\kappa^P_m = \int_{\omega_m}^{\omega_m + \Delta\omega_m} \kappa(\omega) I^P(\omega) d\omega / \int_{\omega_m}^{\omega_m + \Delta\omega_m} I^P(\omega) d\omega,$$

where $I^P(\omega) = \frac{\omega^3 \exp(-\hbar\omega/T)}{1-\exp(-\hbar\omega/T)}$ is the Planck function, $\omega_m$ is the left boundary of the frequency group $m$, $\Delta\omega_m$ is the group width. The Rosseland averaging of the $\beta$ and $\kappa$ coefficients is carried out according to

$$I^R_m = \int_{\omega_m}^{\omega_m + \Delta\omega_m} \frac{1}{\kappa(\omega)} \frac{\partial}{\partial T} I^P(\omega) d\omega / \int_{\omega_m}^{\omega_m + \Delta\omega_m} \frac{\partial}{\partial T} I^P(\omega) d\omega,$$

where $I^R_m$ is the mean Rosseland free path. The Rosseland group opacities $\kappa^R_m$ are obtained from the Rosseland free path according to

$$\kappa^R_m = 1/I^R_m.$$

Common methods (Planck and Rosseland) for averaging of the absorption and emission coefficients can lead to the non-adequate results in radiation transfer calculations for the high-Z element plasma. As it follows from a definition of the procedure of Planck and Rosseland averaging, the Planck averaging leads to an overestimation of the emission in lines which can be very large for coefficients with a lot of splitted and overlapped lines. The procedure of Rosseland averaging results in an underestimation of radiation properties of the high-Z element plasma.

Another approach to obtain the averaged optical properties with a reasonable number of frequency groups is based on the Lebesgue method of integration. The main idea of the Lebesgue method of radiation transfer can be presented as a simple example. Let we have the plasma layer with a constant temperature and density. The frequency range should be divided into several frequency groups of such the width $\Delta\omega_m$ that the Planck function can be assumed to be a constant inside each the group. If this condition is satisfied, any line can be placed in some position within the group, and the absorbed and emitted radiation is not changed. Therefore, the absorption coefficient inside the group can be sorted to produce a monotonic (either increasing or decreasing) function instead of the real one, i.e. so called “equivalent coefficient” is constructed (see Fig. 32). As a result, after this
procedure we have some monotonic quasi-continuum with smooth shape, which can be rather easy approximated. The “equivalent coefficient” is changed inside the group from minimal value \( \kappa_{\text{min}} \) up to maximal value \( \kappa_{\text{max}} \). Inside the group the value of absorption coefficient (from \( \kappa_{\text{min}} \) up to \( \kappa_{\text{max}} \)) is divided into several equidistant sub-intervals \( \Delta \kappa_i = (\kappa_{\text{max}} - \kappa_{\text{min}})/n \). Therefore, the “equivalent coefficient” is approximated by a histogram with use of the equidistant sub-intervals \( \Delta \kappa_i \). The frequency subgroups \( \Delta \omega_{mi} < \Delta \omega_m \) of varied width can be assigned to each sub-interval \( \Delta \kappa_i \). The boundaries of subgroups are determined by intersection points of the “equivalent coefficient” curve with the lines, which are drawn from the \( \Delta \kappa_i \) boundaries in parallel with the frequency axis. The weight of the subgroup \( i \) in the frequency group \( m \) is given as \( \Delta \omega_{mi} / \Delta \omega_m \).

The procedure of Lebesgue averaging requires a modification scheme to calculate the radiation transfer. Within a spatial mesh (mesh size \( \Delta x \) in one-dimensional calculations) with a constant plasma temperature and density, the spectral flux within the group \( m \) (group width \( \Delta \omega_m \)) outgoing from the mesh with the Rosseland and Planck opacities is calculated according to

\[
I_{\text{out}}(m) = I_{\text{in}}(m) e^{-\kappa_s \Delta x} + \frac{\beta_{\omega}}{\kappa_{\omega}} \int_{\Delta \omega_m} I^p(\omega)(1 - e^{-\kappa_s \Delta x}) d\omega,
\]

where \( I_{\text{in}}(m) \) is the incoming spectral flux.

Applying the Lebesgue averaging, the spectral flux within the group \( m \) (\( \omega_m + \Delta \omega_m \)) outgoing from the mesh is calculated according to

\[
I_{\text{out}}(m) = I_{\text{in}}(m) \sum_i \frac{\Delta \omega_{mi}}{\Delta \omega_m} e^{-\kappa_{\omega} \Delta x} + \sum_i \frac{\Delta \omega_{mi}}{\Delta \omega_m} \frac{\beta_{\omega}}{\kappa_{\omega}} \int_{\Delta \omega_m} I^p(\omega)(1 - e^{-\kappa_{\omega} \Delta x}) d\omega,
\]

where \( \beta_{\omega} \) and \( \kappa_{\omega} \) are the equivalent Lebesgue opacity values of the subgroup \( i \) of the width \( \Delta \omega_m \), \( I_{\text{in}}(m) \) is the incoming spectral flux within the frequency group \( m \). Therefore, the radiation is transferred within the frequency groups from mesh to mesh, but inside a mesh the radiation is transferred within the subgroups. For the given frequency group \( m \) the structure of subgroups can be different in the different spatial meshes.

8.1. Description of the tables
The Lebesgue averaged absorption and emission coefficients for the tungsten plasma were produced from the spectral absorption and emission coefficients obtained using 25000 frequency groups (5000 point per order). These tables were calculated for the temperature range 0.5 – 500 eV (20 temperature points per order) and density range 10^{14} – 10^{20} cm^{-3} (2 density points per order).

Four sets of the Lebesgue averaged absorption and emission coefficients were prepared with a varied detail. 21 and 49 frequency group sets are used. For these group sets, two types of division into the sub-groups were applied which give the different number of subgroups within each group. In the first case, the order of absorption coefficient is divided into three intervals (file names: Wlebeg21 and Wlebeg49). In the second case, the absorption coefficient order is divided into six intervals (file names: Wlebeg21a and Wlebeg49a). All the absorption and emission coefficients inside the frequency groups are the “equivalent coefficients” as was defined above.

8.2. Comparison of different averaging types

To validate the statistical radiation transfer method, the test calculations were performed for fixed temperature and density profiles which are typical for a divertor problem (they are shown in Figs. 33, 34). The plasma temperature increases from 1 eV near the divertor plate up to 160 eV at a large distance (about 40 cm), and the density decreases from 10^{19} cm^{-3} up to 10^{12} cm^{-3}, respectively. These profiles were divided into 23 non-uniform spatial meshes. Inside each mesh, the temperature and density are assumed constant. Test calculations include full frequency radiation transfer calculation using both 25000 and 5000 frequency groups, radiation transfer calculation using 18 frequency groups with Planck, Rosseland and Lebesgue averaged absorption and emission coefficients with three points per order (the frequency group scale is the same).

These test calculations allow us: a) to determine convergence of radiation fluxes with increase of a number of frequency groups 5000 → 25000; b) to determine character value of an error for Planck and Rosseland mean coefficients in assumption that for 25000 frequency groups a calculation is standard; c) to determine a degree of accuracy of the Lebesque method.

Radiation transfer problem is solving using an integral radiation transfer equation described above for the Planck-Rosseland and Lebesgue averaging.

Results of test calculations are described below. The radiative fluxes onto the wall and back-radiated obtained using 5000 and 25000 frequency groups are
shown in Figs. 35-38. A difference between the results with different detail of frequency resolution does not exceed 10-15 %. Radiative fluxes onto the wall and back-radiated obtained using the mean Planck and Rosseland coefficients and the Lebesgue method are shown in Figs. 39, 40, respectively.

The used temperature and density profiles correspond some exact time moment. It is evident that for another time moments the spatial size of plasma region, temperature and density distributions is changed. To understand how the radiative fluxes obtained using different opacity would change in rather different situation, the scaling of spatial size is applied. By this way, one can simulate both optically thin and optically thick plasmas. The spatial meshes were uniformly scaled $\Delta x = C \cdot \Delta x$. The scaling factor was chosen in the range $0.01 < C < 1000$ with the step of 3. A comparison of integral radiative fluxes onto the wall and back-radiated obtained by means of the different methods is shown in Fig. 41 and 42, respectively.

From the comparison, we can make the following conclusions. The Lebesgue method gives more advantages for radiative fluxes onto the wall in comparison with the Planck and Rosseland ones. A deflection from the standard result (25000 frequency groups) is smaller. The back-radiated fluxes obtained using the Lebesgue method are also more closed to the standard one in comparison with the fluxes obtained using the averaged Planck and Rosseland opacities for the case of optically transparent and semi-transparent plasma. The Lebesgue method and averaged Rosseland opacities give comparable results for the optically thick plasma and sometimes the Rosseland opacities are accurate. This is because the absorption coefficients in the Lebesgue method are determined with a rather low accuracy (3 points per order). In case of more detailed division of the absorption coefficient scale (6 points per order), the accuracy of the Lebesgue results is increased. The results are also shown in the Figs. 41, 42. The name of corresponding curves is New Lebesgue.
FIG. 28  TUNGSTEN PLASMA  \( T=17.74 \text{ eV} \)  \( N=10^{17} \text{ cm}^{-3} \)

FIG. 29  TUNGSTEN PLASMA  \( T=17.74 \text{ eV} \)  \( N=10^{17} \text{ cm}^{-3} \)
Fig. 30 Balance of tungsten plasma. $N = 10^{16} \text{cm}^{-3}$

Fig. 31 Balance of tungsten plasma. $N = 10^{18} \text{cm}^{-3}$
FIG. 32 TUNGSTEN PLASMA  T=17.74 eV  N=10^{17} cm^{-3}

FIG. 33 TUNGSTEN PLASMA  PROFILE OF TEMPERATURE
Fig. 34 TUNGSTEN PLASMA PROFILE OF DENSITY

Fig. 35 EMISSION SPECTRUM OF TUNGSTEN PLASMA
Fig. 36  EMISSION SPECTRUM OF TUNGSTEN PLASMA

Fig. 37  EMISSION SPECTRUM OF TUNGSTEN PLASMA
Fig. 38 EMISSION SPECTRUM OF TUNGSTEN PLASMA

Fig. 39 EMISSION SPECTRUM OF TUNGSTEN PLASMA
Fig. 40 EMISSION SPECTRUM OF TUNGSTEN PLASMA

Fig. 41 COMPARISON DIFFERENCE METHOD OF TRANSFER
Fig. 42 COMPARISON DIFFERENCE METHOD OF TRANSFER
References