

Excitation of highly-lying atomic states: project and first results

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Abstract

The project is aimed at calculation of the cross-sections and rates for electron impact excitation for levels up to $n=10$ for atoms and their ions with $Z \leq 26$, and preparing the diagnostic tools for analysis of the spectra of the astrophysical sources using the obtained atomic parameters. As a main instrument of the calculations we plan to use some versions of the Distorted Wave approximation, that we consider optimal, including effects of exchange and configuration interaction when necessary. The first results obtained in the framework of the project - the cross sections and effective collision strengths for electron impact excitation of considered ions are presented. The impact of the excitations into the high-lying states on the intensity of the C, N and O ion lines in the spectra of low-density plasma and the cooling rates for these ions are demonstrated.

1 Introduction

The electron-impact excitation of highly-lying atomic levels can give a great contribution to the intensities of the UV, optical and IR lines observed in the spectra of various types of the astrophysical sources. For modelling the spectra of these objects and obtaining their parameters from comparison of observed and calculated lines and continuum intensities we need a lot of atomic data. The main bulk of those parameters are the transition probabilities (oscillator strengths) and electron impact excitation cross sections (rates of excitation by electron impact).

The majority of the atomic data which are presented in the literature, in the atomic data catalogue and databases (see, for example, [6, 11]) refer to the ground and low lying states. At the same time, for calculating the spectra of the astrophysical sources the rates of radiative and collision transitions between highly-lying atomic and ionic states are necessary.

Here we present the project HILYS (**H**ighly **L**ying **S**tates) aimed at obtaining the atomic parameters of such states for atoms and their ions. The main purpose of the project is calculation of the cross-sections and rates for electron impact excitation for levels up to $n=10$ for atoms and their ions with $Z \leq 26$. We also plan to construct the diagnostic tools for obtaining the parameters of the emitting plasma from the observed line intensities in the spectra of astrophysical sources. In this report we present the scope of the project and the first results. Some previous results can be also found in our recent papers [3, 13].

2 Methods of calculation

Today the methods are developed that permit to obtain probably all characteristics of the scattering process with high accuracy. We have in mind the R-matrix [1] and Convergent Close Coupling (CCC) [5] methods, that make use of big basis sets of pseudofunctions. But these methods require so big computing resources that up to now calculations have been done only for effectively one- and two-electron targets. As for our project we need a great number of cross sections for different atoms and ions, we have to use simpler theories, but try to understand clearly the area of their validity.

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We have accepted as the main method the method of distorted waves (DW approximation), which permits to asses reasonably the cross sections for many processes of excitation for atoms and ions. More then that. For the integral excitation cross sections of neutral atoms we find it useful even simple Born approximation (with modification [2] for exchange), as the DW approximation for such problems is better then simple Born mostly for description of differential cross sections.

Below we remind general formulae and explain the notations in the figures.

3 Wave functions of the bound and free electrons

In our program the target wave functions are built as antisymmetrized combinations of one electron functions, which in their turn are defined as eigenfunctions of one electron Schroedinger equation with appropriate potential, or from the solution of Hartree-Fock equations.

In the first case it is easy to achieve the mutual orthogonality of the initial and final bound wave functions, and, after calculating in the same potential the functions describing the incoming and scattered electrons, to obtain also their orthogonality to the bound ones. This last property is important for correct account of exchange effects at low energies.

In the second case the wave functions of initial and final states of the target are orthogonalized and then considered as basis on which the energy operator of the target is diagonalized. Such solutions are also mutually orthogonal and in this scheme configuration interaction approximation can be realized. But for free states artificial orthogonalization was applied.

4 General Formulae

$$H = H_0 + H_{at} + V \quad (1)$$

$$H_0 = -1/2\nabla_0^2 \quad (2)$$

$$H_{at} = \sum_{i=1}^N \left(-1/2\nabla_i^2 - Z/r_i \right) + \sum_{i<j=1}^N 1/r_{ij} \quad (3)$$

$$V = V(\mathbf{r}_0, \mathbf{X}) = e^2 \left(Z/r_0 - \sum_{i=1}^N 1/r_{0i} \right) \quad (4)$$

$$H_{at}\phi_n = \varepsilon_n\phi_n \quad \sum_n |\phi_n\rangle\langle\phi_n| = 1 \quad (5)$$

$$H\Psi_a^+ = E\Psi_a^+ \quad \Psi_a^+ \sim \exp(i\mathbf{k}_a\mathbf{r}_0)\phi_a(\mathbf{X}) + scatt.waves \quad (6)$$

$$f_{ba}(k_b, k_a) = -\frac{1}{2\pi} \langle k_b\phi_b | V | \Psi_a^+ \rangle = \quad (7)$$

$$= -\frac{1}{2\pi} \int \exp(-i\mathbf{k}_b\mathbf{r}_0)\phi_b^*(\mathbf{X})V(\mathbf{r}_0, \mathbf{X})\Psi_a^+(\mathbf{r}_0, \mathbf{X})d\mathbf{r}_0d\mathbf{X} \quad (8)$$

$$\frac{d\sigma_{ba}}{d\Omega} = \frac{k_b}{k_a} |f_{ba}(\mathbf{k}_b, \mathbf{k}_a)|^2 \quad (9)$$

$$\sigma_{ba} = \int \frac{d\sigma_{ba}}{d\Omega} d\Omega \quad (10)$$

$$\sigma_{total} = \sum_b \sigma_{ba} = \frac{4\pi}{k_a} \text{Im} f_{aa}(\vartheta = 0) \quad (11)$$

$$\mathbf{q} = \mathbf{k}_a - \mathbf{k}_b \quad q^2 = k_a^2 + k_b^2 - 2k_a k_b \cos \vartheta \quad (12)$$

$$q dq = k_a k_b \sin \vartheta d\vartheta \quad (13)$$

4.1 First Born Distorted Wave Approximation (DWB1)

If

$$V = V_1(\mathbf{r}_0) + V_2(\mathbf{r}_0, X) \quad (14)$$

and

$$(K_0 + V_1)\psi_{k_a}^{\pm}(\mathbf{r}) = 0 \quad (15)$$

then in DW approximation $\Psi_a(r_0, X)$ is put equal to

$$\Phi_a^{pm}(\mathbf{r}_0, X) = \psi_{k_a}^{\pm}(\mathbf{r}_0)\phi_a(X) \quad (16)$$

It can be substituted into (8), but much more consistent approximation [4, 17] can be obtained rewriting (8) by the Gell-Mann and Goldberger "two-potential formula" what results in

$$2\pi f_{ba}^{dir}(\mathbf{k}_b, \mathbf{k}_a) = - \langle \psi_{k_b}(r_0)\phi_b(r_1, \dots, R_N) | V_1(\mathbf{r}_0) | \Phi_a^+(\mathbf{r}_0, X) \rangle - \langle \Phi_b^-(\mathbf{r}_0, X) | V_2(\mathbf{r}_0, X) | \Phi_a^+(\mathbf{r}_0, X) \rangle \quad (17)$$

for direct part of the scattering amplitude, and

$$2\pi f_{ba}^{exch}(\mathbf{k}_b, \mathbf{k}_a) = - \langle \psi_{k_b}(r_1)\phi_b(r_0, \dots, R_N) | V_1(\mathbf{r}_0) | \Phi_a^+(\mathbf{r}_0, X) \rangle - \langle \Phi_b^-(\mathbf{r}_1, r_0, r_2, \dots, r_N) | V_2(\mathbf{r}_0, X) | \Phi_a^+(\mathbf{r}_0, X) \rangle \quad (18)$$

for the exchange one

For the inelastic scattering matrix element with V_1 in direct part of the scattering amplitude is zero because of orthogonality of atomic states ϕ_a and ϕ_b .

For the exchange one this is so only when free states ψ_k are either calculated in the same potential as atomic wave functions, or artificially made orthogonal to them.

It seems very natural not to have contribution to the exchange part of the scattering amplitude from the interaction with the core. This idea was advocated by Day et al. [4], but was not accepted by the atomic collision community, may be because of the habit not to have functions with coulomb asymptotic behavior for neutral targets.

But simple antisymmetrization led often to unrealistically big increase of the exchange amplitude. So, forced orthogonalization became popular. It was mostly used only for f_{ab}^{exch} and its influence on the f_{ab}^{dir} is not stressed. But the scattering amplitude is a single whole and such a procedure cannot be regarded as a satisfactory solution.

Below on some simple examples of direct and exchange transitions in H and He we tried to demonstrate the effects of "forced" and "natural" orthogonalization. We hope the results are not widely recognized. But they should be investigated whenever one wants to use the DW approximation.

At the present stage of the project we have programs to calculate target and free wave functions, Born and different versions of DW integral and differential cross sections and collision rates. We

are in the stage of accumulating experience, comparing the results of our calculations with those available in the literature. For this seminar we present several results demonstrating the role of forced and natural orthogonalization which we believe are not clearly appreciated.

We also show the case of $1s^1S - 2s^3S$ transition in He for which also CCC (I.Bray) result is given and an example of first order DW result for differential cross section for $1s - 2s + 2p$ transition in atomic hydrogen for which new experiment is available and compared with CCC and Madison second order DW calculations [8].

To finish with let us explain (on example of H atom) notations in the figures connected with different choices of distorting potential:

The curves are labeled as:

Born approximation - B

EP - for DW approximation with distorting potential same, as seen by active atomic electron

DW approximation - distortion potential AP1:

$$V_1(r_0) = \left\langle \phi_a \left| \frac{Z}{r_0} - \frac{1}{r_{01}} \right| \phi_a \right\rangle \quad (19)$$

AP1 NN - distortion potential AP1, No orthogonalization, No exchange.

AP1 YN - distortion potential AP1, with orthogonalization, but no exchange and so on.

AP2 - for DW approximation with distortion potential (recommended by D.Madison [12]):

$$V_1(r_0) = \left\langle \phi_b \left| \frac{Z}{r_0} - \frac{1}{r_{01}} \right| \phi_b \right\rangle \quad (20)$$

AP2 NN, AP2 YN, AP2 YY have the same meaning as for AP1: first letter N or Y means account for orthogonalization, second - for exchange.

5 Plasma diagnostics

The problem of the plasma diagnostics is a determination of the plasma parameters: atom and ion density and temperature distribution over the all emitting volume. Here we consider the case of the optically thin in the line frequencies (excluding in some case the line of the resonance transitions) medium.

5.1 Diagnostic of the homogeneous plasma

For the sake of the simplicity we consider only the lines controlled by electron collisions and photo and dielectronic recombinations. The total energy emitted by the studied object in a recombination or collisionally excited line $k \rightarrow i$ of the ion X is

$$E_{ki} = h \nu_{ki} \int_V n_F r_{ki}^{\text{eff}} dV. \quad (21)$$

Here ν_{ki} is the frequency of the line; V is the total volume of the region emitting in the line; $n_F = n(X_F)$ is the number density of the ion X_F , which is responsible for the formation of the line. For collision lines $X_F \equiv X$, but for recombination ones $X_F \equiv X^+$. The coefficient r_{ki}^{eff} is known as

the effective line formation coefficient (see [16]). In the case of recombination lines, $r_{ki}^{\text{eff}} = n_e \alpha_{ki}^{\text{eff}}$, where n_e is the electron number density and α_{ki}^{eff} is the effective recombination coefficient of the line. For collision lines, $r_{ki}^{\text{eff}} = n_e q_{ki}^{\text{eff}}$. Here q_{ki}^{eff} is the effective coefficient of the collision excitation for the line $k \rightarrow i$, determined in such a way that $(4\pi)^{-1} n_e n(X) q_{ki}^{\text{eff}}$ is the emission coefficient of the line.

In the homogeneous case plasma diagnostics reduces to determination of mean electron temperature and density and the partial ion abundances:

$$X_{ij} = (N_{ij})/N_j, \quad N_j = A_j * N, \quad (22)$$

where N_{ij} is a number density of ion i of element j , A_j is a relative element j abundance.

$$E_{ki} \approx E_{ki}^0 = h \nu_{ki} r_{ki}^{\text{eff}}(T_0, n_e^0) \int_V n_F dV = h \nu_{ki} r_{ki}^{\text{eff}}(T_0, n_e^0) N_F, \quad (23)$$

where N_F is the total number of the ions X_F . The value of T_0 has been determined by [14] and [15]:

$$T_0 = \int_V T_e n_e n_F dV / \int_V n_e n_F dV. \quad (24)$$

More elaborately the methods of homogeneous plasma diagnostics are consider in [16]. It should be mention that the values of n_e^0 and T_e^0 obtained from line intensities of different ions can be strongly different. This differences are connected mainly with the temperature and density fluctuations inside the emitting volume. The impact of such fluctuations on the line intensities and plasma diagnostics is considered in the next subsection.

5.2 Diagnostic of the inhomogeneous plasma

Here we consider both the temperature and density fluctuations in the linear approximations. Instead of the values of T_e and n_e we can use the dimensionless parameters

$$t = T_e/10^4\text{K}; \quad s = \lg(n_e) + \alpha.$$

where parameter $\alpha = 0 - 2$.

Let us suppose that the values of the temperature and electron number density fluctuations are small relatively to the values of T_e and n_e and determine the mean (for the considered ion, which is responsible for the line formation) values of the parameters:

$$\langle t \rangle_F = \bar{t} = \int_V t n_F dV / \int_V n_F dV = \int_V t n_F dV / N_F \quad (25)$$

and

$$\langle s \rangle_F = \bar{s} = \int_V s n_F dV / \int_V n_F dV = \int_V s n_F dV / N_F. \quad (26)$$

Let us determine the following parameters describing the *rms* fluctuations of T_e and n_e :

$$\tau^2 = \frac{\int_V (t - \bar{t})^2 n_F dV}{\bar{t}^2 N_F}, \quad (27)$$

$$\boldsymbol{\tau\sigma} = \frac{\int (t - \bar{t})(s - \bar{s}) n_{\text{F}} dV}{\bar{t} \bar{s} N_{\text{F}}}, \quad (28)$$

$$\boldsymbol{\sigma^2} = \frac{\int (s - \bar{s})^2 n_{\text{F}} dV}{\bar{s}^2 N_{\text{F}}}. \quad (29)$$

In the linear approximation for small amplitude fluctuations of T_e and n_e , the total line intensity can be presented in the form:

$$E_{ki} = E_{ki}^0 (1 + \mu_{tt} \boldsymbol{\tau^2} + \mu_{ts} \boldsymbol{\tau\sigma} + \mu_{ss} \boldsymbol{\sigma^2}) \quad (30)$$

Where E_{ki}^0 is described by expression (23). The parameters μ_{tt} , μ_{ts} and μ_{ss} are determined by the following expressions:

$$\mu_{tt} = \left[\frac{1}{2} \frac{\partial^2 r_{ki}^{\text{eff}}}{\partial t^2} (r_{ki}^{\text{eff}})^{-1} t^2 \right]_{t=\bar{t}; s=\bar{s}}, \quad (31)$$

$$\mu_{ts} = \left[\frac{\partial^2 r_{ki}^{\text{eff}}}{\partial t \partial s} (r_{ki}^{\text{eff}})^{-1} t s \right]_{t=\bar{t}; s=\bar{s}}, \quad (32)$$

$$\mu_{ss} = \left[\frac{1}{2} \frac{\partial^2 r_{ki}^{\text{eff}}}{\partial s^2} (r_{ki}^{\text{eff}})^{-1} s^2 \right]_{t=\bar{t}; s=\bar{s}}. \quad (33)$$

By using the parameter s instead of the value of n_e we can describe the significant (up to 2 times) deviations on the mean electron number density in the linear approximation.

The dependencies of the parameters μ_{tt} , μ_{ts} and μ_{ss} on T_e and n_e for OIII lines are plotted in the Figs. D1 and D2. As this figures shows the coefficients μ_{ts} and μ_{ss} are well below the μ_{tt} . Only for the high density nebulae ($n_e > 10^4 \text{cm}^{-3}$) the contribution of the electron number density variations in the total line intensities can be essential.

5.3 Determination of the plasma parameters

We use an empirical model of a emitting object (in this paper – planetary nebulae) to find the plasma parameters from the observed line intensities. In this model the object is described by its mean electron temperature T_0 , mean electron number density n_e^0 and *rms* temperature and electron number density fluctuations $\boldsymbol{\tau^2}$ and $\boldsymbol{\sigma^2}$ as well as the correlation parameter $\boldsymbol{\tau\sigma}$. The relative element abundances are assumed to be constant in the whole volume of the nebula.

In general each ion X^{n+} has to be described by its own values of plasma parameters $T_0(X^{n+})$, $\bar{s}(X^{n+})$, $\boldsymbol{\tau^2}(X^{n+})$, $\boldsymbol{\tau\sigma}(X^{n+})$ and $\boldsymbol{\sigma^2}(X^{n+})$. However, as numerous calculations have shown those parameters for ions with the similar ionization potentials are very close, so we do not consider these differences. Finally we list the parameters of the model: T_0 , \bar{s} , $\boldsymbol{\tau^2}$, $\boldsymbol{\tau\sigma}$, $\boldsymbol{\sigma^2}$ and $\{N(X)/H\}$ – the relative abundances of elements.

The atomic data which are necessary for line intensities were taken from the catalogue [6], databases, cited in [11] or were calculated in the framework of the considered project. The contribution of both the photo and dielectronic recombination into the total effective recombination coefficients has been taken into account. For fitting the calculated and observed line intensities we use the procedure proposed in [9, 10]. This procedure is illustrated in Fig. D3.

6 Cooling rates for inhomogeneous plasma

One of the most important parameters of the plasma is its cooling rate. This value – L is determined as an energy, emitted by the unit volume in the unit time. We consider an optical thin plasma, controlled by the collisions of atoms and ions with electrons. In this case the local cooling rate is determined by local electron temperature and density of the medium. We can express the cooling rate in term of the so named "cooling function" $\Lambda = L/n^2$, where n is the total number density. Using the partial ion abundances X_{ij} determined by the equation 22 we find:

$$\Lambda = \sum_{ij} X_{ij} \lambda_{ij}, \quad (34)$$

where λ_{ij} is the partial cooling function:

$$\lambda_{ij} = \sum_{kl} n_k h\nu_{kl} A_{kl} \quad (35)$$

6.1 Ionization equilibrium

For finding the total cooling function we need the distributions of atom on their ionization states. Those are determined by solving the equations of the ionization equilibrium:

$$\frac{x_{i-1j}}{x_{ij}} = \frac{\alpha_{ij}(T)}{C_{i-1j}(T)}, \quad (36)$$

where α_{ij} is the total recombination rate for ion i of atom with number j and C_{ij} is the collision ionization rate for the same ion together with condition

$$\sum_{j=0}^Z x_{ij} = 1, \quad (37)$$

where $Z = Z(j)$ is the atomic number of element j .

The typical dependencies of the relative ionic abundances are presented in Fig. D4 for O ions. The sources of the atomic data are described in the previous section.

6.2 Results

As an example, we have calculated the cooling functions both for homogeneous and inhomogeneous plasma. The solar abundances of elements were taken from [7]. In Fig. D5 is presented the cooling functions for H+He+O mixture both for solar abundances and for values of 0.1 and 10.0 of them. One can see that in the presence of temperature fluctuations the cooling function can strongly exceed its value for homogeneous plasma. It means, that the cooling times for inhomogeneous plasma are less then homogeneous one.

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Fig. 1. Cross sections for electron impact excitation of transition 1s-2p HI.

Fig. 2. The same as in Fig. 1, but for ion He II.

Fig. 3. The same as in Fig. 1, but for ion Be IV.

Fig. 4. The same as in Fig. 1, but for ion Ne X.

Fig. 5. The same as in Fig. 1, but for transition 1s-3p HI.

Fig. 6. The same as in Fig. 1, but for transition 1s-5p HI.

Fig. 7. The same as in Fig. 1, but for transition $1s\ ^1S - 1s\ ^3S$ HeI.

Fig. 8. The parameters μ_{tt} , μ_{ts} , and μ_{ss} for the [OIII] λ 5007 line as a function of T_e (upper panel) and n_e (lower panel).

Fig. 9. The same as in Fig. 1 but for the [OIII] $\lambda 88 \mu m$ and $\lambda 52 \mu m$ lines.

Fig. 10. Line fitting for planetary nebula NGC 7027. Calculated line intensities (solid lines) are normalized to the observed ones. The dashed line represents the probability distribution function normalized to its maximal value. Upper panel: T_e fit, lower panel: n_e fit

Fig. 11. The dependencies of the relative abundances of oxygen ions on electron temperature T_e in low-density plasma.

Fig. 12. Upper Panel: cooling function ($\text{eV s}^{-1} \text{cm}^{-6}$) for H+He+O and $\tau^2 = 0.01, 0.02, 0.04, 0.08, 0.16$ (from bottom to top). Lower Panel: the same as in upper panel, but for different oxygen abundances (Z/Z_{sun}) relatively the solar value ($7.4 \cdot 10^{-4}$).