Plasma effects on the atomic structure and X-ray lines of astrophysical interest. The case of oxygen ions

J. Deprince [1], **P. Palmeri** [1], **P. Quinet** [1,2]

[1] Physique Atomique et Astrophysique, Université de Mons, B-7000 Mons, Belgium
[2] IPNAS, Université de Liège, B-4000 Liège, Belgium

The main goal of the present work is to estimate the effects of plasma environment on the atomic parameters associated with the K-vacancy states in astrophysically important oxygen ions within the context of accretion disks around black holes. In order to do this, relativistic atomic structure calculations are carried out by considering a time-averaged Debye-Hückel potential for both the electron-nucleus and electron-electron interactions. A first sample of results related to the ionization potentials, the transition energies and the radiative emission rates is reported for all the ionization stages of oxygen, from O I to O VII.

Introduction

An atom bombarded by X-rays can undergo an ionization in which an inner-shell electron is ejected. The system can thus deexcite itself by an electronic transition in which an outer electron fills this vacancy. The available energy associated to this transition can lead (among other possibilities) to the emission of an X-ray photon by the atom (X-ray fluorescence). Such a transition in which the inner-shell involved in the process is characterized by the principal quantum number $n = 1$ is called a K-line.
X-ray K-lines emitted by cosmologically abundant ions, such as oxygen and iron ions, play an essential role in astrophysics. Iron and oxygen K-lines have actually been observed by the high-resolution X spectrometers on board the *XMM-Newton*, *Chandra* and *Suzaku* satellites in numerous astrophysical spectra of objects such as AGN, galactic black holes, supernova remnants, X-ray binaries or neutron stars (see, for example, [1], [3], [2], and [4]).
In particular, in most accreting black hole or neutron star systems, the hard X-rays emitted from the inner-most regions can be reprocessed by the accretion disk. In the resulting so-called "reflection" spectrum, the fluorescence K-lines from iron and oxygen are the most prominent lines ([5], [6], [7], [8]) and are of great interest

since they can be considered as very useful natural probes for studying accreting black holes [9]. Actually, they can be grossly broadened and skewed due to Doppler effects and gravitational redshift ([5], [10]), so that fitting a model reflection spectrum over the observed one allows to measure the black hole spin among other physical quantities ([11], [12]). The black hole spin, in particular, can be measured by estimating from the fit the radius of the accretion disk inner edge, which is supposed to be located at the innermost stable circular orbit (*ISCO*), since the *ISCO* radius simply and monotonically maps to the black hole spin [13]. Consequently, very accurate iron and oxygen atomic data related to K-vacancy states are absolutely required to model at best the X-ray fluorescence lines appearing in the reflection spectrum of a black hole accretion disk.

However, the accuracy of the physical quantities, such as the black hole spin, when measured in this way from iron lines, is called into question since fitting the data over the model spectrum requires uncommonly high iron abundances ([14], [15]), namely several times the solar value. Since no plausible physical explanation of these super-solar iron abundances is known, the most likely explanation is a deficiency in the current models. This lack should mainly arise from the validity of the atomic data used in the models, as these latter merely include atomic parameters corresponding to isolated ions and therefore may not be applicable at very high densities. Indeed, in real astrophysical circumstances, emitting ions are embedded in a rather dense plasma forming the accretion disk. By the way, recent magnetohydrodynamics simulations tend to support the existence of a relatively high density in black hole accretion disks. More precisely, in a recent analysis [16], American scientists estimate that the plasma physical conditions in a typical black hole accretion disk should be characterized by a temperature ranging from 10^5 K to 10^7 K and an electron density ranging from 10^{18} cm^{-3} to 10^{21} cm^{-3}. Therefore, and as recently mentioned in a review entitled *Atomic Data Needs for Understanding X-ray Astrophysical Plasmas* [17], for a reliable interpretation of accretion disk X-ray spectra, it is crucial to consider the high-density plasma effects in the calculation of the atomic data implemented in the models.

In this work, we present an estimate of the plasma environment effects on the ionization potentials and radiative parameters for all the ionization stages of oxygen. The choice of oxygen is motivated by the smaller number of different ions and by the simpler atomic structures compared to iron ions. In this way, a complete and consistent model of atomic data related to K-vacancy states in all the oxygen ions, taking the plasma environment into account, can be more easily achieved than for iron ions.

Atomic structure calculations

In this work, two independent theoretical methods are used to model the atomic structures and to compute the radiative parameters, namely the purely relativistic multiconfiguration Dirac-Fock (MCDF) method, by using a combination of the GRASP92 [18] and of the RATIP [19] codes, and the Breit-Pauli relativistic approximation as implemented in the AUTOSTRUCTURE code ([20], [21]).

In the MCDF approach, all the atomic state functions (ASFs), $\Psi(\gamma, P, J, M_J)$, are expanded in linear combinations of configuration state functions (CSFs) of the same parity (P) and total angular momentum (J, while M_J denotes its projection), $\Phi(\alpha_i, P, J, M_J)$, that is

$$\Psi(\gamma, P, J, M_J) = \sum_i c_i \, \Phi(\alpha_i, P, J, M_J) \,. \qquad (1)$$

The CSFs are in turn built as antisymetrized products of orthonormal monoelectronic spin-orbitals of the form

$$\varphi_{n\kappa m}(r, \theta, \phi) = \frac{1}{r} \begin{pmatrix} P_{n\kappa}(r) \, \chi_{\kappa m}(\theta, \phi) \\ iQ_{n\kappa}(r) \, \chi_{-\kappa m}(\theta, \phi) \end{pmatrix} , \qquad (2)$$

where $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are, respectively, the large and the small component of the radial wavefunction, and the angular functions

$\chi_{\kappa m}(\theta, \phi)$ are the spinor spherical harmonics. The quantum number κ is given by $\kappa = \pm(j + 1/2)$, where j is the electron total angular momentum quantum number and where the sign is chosen in such a way that it corresponds to the coupling relation between the electron orbital momentum, l, and its spin, *i.e.* $l = j \pm 1/2$. The radial functions $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ and the expansion coefficients c_i are optimized self-consistently by resolving numerically the MCDF equations that arise from a variational principle. The computations are completed with the inclusion of the relativistic two-body Breit interaction and the quantum electrodynamic corrections (QED) due to self-energy and vacuum polarization. The MCDF wavefunctions generated by the GRASP92 code are then used in the RATIP program to compute the atomic structure and the radiative parameters associated with the K-vacancy states.
In order to obtain the MCDF multiconfigurational expansions for all the polyelectronic oxygen ions (O I - O VII), the active space (AS) method is used. This latter consists in exciting some electrons from the reference configurations to a given set of excited state orbitals. For each oxygen ion, the AS is built by considering all the single and double excitations from the configurations involved in the K-shell transitions. This gives rise, depending on the ion, to a number of CSFs ranging from 98 to 7389.
In the AUTOSTRUCTURE method, the wavefunctions are built by using single-electron orbitals generated from a scaled Thomas-Fermi-Dirac-Amaldi (TFDA) potential. The scaling parameters for each orbital are optimized in a multiconfiguration variational procedure minimizing a weighted average of non-relativistic contributions to the energy. Spin-orbit coupling and Breit-Pauli operators are introduced as perturbations to obtain fine-structure relativistic corrections. It is important to mention that this method is mainly used by our collaborators from the California Institute of Technology (J. Garcia), the NASA Goddard Space Flight Center (T. R. Kallman) and the Western Michigan University (M. Bautista, C. Mendoza) within the framework of a NASA-APRA proposal in which our research unit is involved.

Plasma effect modeling

In a plasma, the electrostatic potential created by an ion is influenced by the plasma free electrons and nearby ions. As a result, not only the atomic structure of the ion is modified (shift of the energy levels and wavelengths, line broadening) but also the ionization potential is lowered. More generally, depending on the plasma conditions, electrostatic potential screening effects can influence all the radiative and non-radiative parameters and can therefore modify physical properties which are essential to the environment description such as opacity, ionization balance and equation of state.
A plasma environment can be classified into weakly and strongly coupled plasma depending on the strength of its coupling parameter Γ, defined as the ratio of the coulombian potential interaction energy between two particles of the plasma to the thermal energy :

$$\Gamma = \frac{e^2}{4\pi\varepsilon_0 d k T_e}, \tag{3}$$

where d is the typical distance which separates these two particles, that is

$$d = \left(\frac{3}{4\pi n_e}\right)^{1/3}, \tag{4}$$

T_e is the electronic temperature of the plasma and n_e is the plasma electron density. The plasma coupling parameter depends thus only on the physical conditions within the plasma (T_e and n_e). For conditions such as $\Gamma \ll 1$, the plasma environment can be considered as weakly coupled, whereas a plasma is classified as strongly coupled if $\Gamma \gg 1$.
For typical conditions characterizing the accretion disk of a black hole (see the discussion above), the plasma forming the disk material can be considered as a weakly coupled plasma, since its coupling parameter Γ ranges from 2.7×10^{-5} to 0.27 (the latter value corresponding to the most "extreme" case, namely the

lowest temperature combined with the highest electron density).

In the case of a weakly coupled plasma, the plasma screening effects on atomic properties can be modeled by considering a Debye-Hückel potential (instead of a coulombian one) for both the electron-nucleus and electron-electron interactions, which can be expressed (in atomic units) as

$$V^{\mathrm{DH}}(r,\lambda) = -\sum_{i=1}^{N} \frac{Ze^{-\lambda r_i}}{r_i} + \sum_{j<i}^{N} \frac{e^{-\lambda r_{ij}}}{r_{ij}} \quad \text{(a.u.)}, \tag{5}$$

where N is the number of bound electrons, r_i is the distance of the ith electron from the nucleus, and r_{ij} is the distance between the electrons i and j. The plasma screening parameter, λ, is the inverse of the Debye shielding length, λ_{De}, and can be expressed, in atomic units, in terms of the physical conditions in the plasma as

$$\lambda = \frac{1}{\lambda_{\mathrm{De}}} = \left(\frac{4\pi n_e}{kT_e}\right)^{1/2} \quad \text{(a.u.)}. \tag{6}$$

Hence, any given values of both the temperature and the electron density of the plasma correspond to a certain value of the screening parameter λ. In the astrophysical context of an accretion disk around black hole, the physical conditions discussed above correspond to screening parameter values up to about 0.1 a.u., whereas the isolated ion case corresponds obviously to $\lambda = 0$ a.u. For these reasons, in our work, the plasma environment effects are estimated by means of a Debye-Hückel potential with a screening parameter λ ranging from 0 to 0.1 a.u.

Results and astrophysical implications

The effects of the plasma environment on the ionization potential (IP) of all the oxygen ions are shown in the table displayed in Figure 1. In this table, the IP of each oxygen ion computed by both the MCDF/RATIP and the AUTOSTRUCTURE methods is given for the plasma screening parameter values $\lambda = 0$ a.u. (isolated ion case) and $\lambda = 0.1$ a.u. The NIST values [22] are also given for comparison. As one can see by looking at this table, when going from $\lambda = 0$ a.u. to $\lambda = 0.1$ a.u., the ionization potential of each ion is lowered by several eV, and this lowering raises with the ionization stage (*i.e.* as the number of bound electrons decreases). Moreover, one can note that the results obtained by both theoretical methods are in excellent agreement concerning the relative effect of the plasma on the IP for each oxygen ion. Let's also point out that the magnitude of the K-threshold (*i.e.* the K-shell ionization limit) lowering for each ion is almost the same (within less than 1%) as the ionization potential one. The fact that the IPs computed by AUTOSTRUCTURE are closer to the NIST values than the ones obtained by MCDF/RATIP can be explained by the different models and strategies used to optimize the orbitals in the two approaches. While our AUTOSTRUCTURE computation is focused on the ground states (giving very accurate IPs), the MCDF/RATIP one is more global (optimizing a weighted trace of the Hamiltonian) in order to describe at best the high-lying K-vacancy states (providing thus more accurate K-line radiative wavelengths).

However, the effects of the plasma environment on the K-line radiative parameters are rather small. This is illustrated in Figure 2 which shows the plasma effects on the wavelengths of two K-lines in O IV and in Figure 3 which displays the sensitivity of the radiative transition probabilities to the screening parameter for two K-lines in O III. More precisely, for $\lambda = 0.1$ a.u. and for each ion, all the K-line wavelengths are redshifted by 10^{-2} Å to 10^{-3} Å compared to the isolated ion, which corresponds to a relative variation of less than 0.1%. In the same conditions of plasma environment and for each ion, the radiative rates of all the K-lines are reduced by about 1% on average (and the variation does not exceed a few percent for a very few transitions). The plasma environment effects on K-line radiative parameters in a material with such physical conditions (corre-

Ion	NIST	MCDF/RATIP			AUTOSTRUCTURE		
	IP (eV)	IP (λ = 0.0) (eV)	IP (λ = 0.1) (eV)	ΔIP (eV)	IP (λ = 0.0) (eV)	IP (λ = 0.1) (eV)	ΔIP (eV)
O I	13.62	12.54	9.93	-2.61	13.62	11.20	-2.42
O II	35.12	33.02	27.74	-5.28	35.17	30.14	-5.03
O III	54.94	52.34	44.46	-7.88	54.85	47.18	-7.67
O IV	77.41	74.48	63.99	-10.49	77.67	67.32	-10.35
O V	113.90	111.44	98.37	-13.07	113.83	100.87	-12.96
O VI	138.12	135.71	120.06	-15.65	137.75	122.13	-15.62
O VII	739.33	737.47	718.59	-18.88	738.89	720.12	-18.77

Figure 1: *Plasma effects on the ionization potential (IP) of all the oxygen ions computed by MCDF/RATIP and AUTOSTRUCTURE. The NIST values [22] are also given. ΔIP = IP($\lambda = 0.1$)−IP ($\lambda = 0.0$).*

sponding to typical accretion disk conditions) are thus rather small and can be neglected in the modeling of astrophysical spectra.

The lowering of several eV observed for the ionization potentials and the K-thresholds of each oxygen ion in typical physical conditions encountered in an accretion disk around a black hole has nevertheless important astrophysical implications that have to be considered in the modeling of the reflection spectrum emitted by the disk. First of all, such a continuum lowering may imply some modifications in the ionization balance and, thus, on the oxygen ionization stages present in the plasma compared to what could be predicted by using the IP values calculated in the isolated ion case. Also, as the initial K-vacancy states of K-lines observed in the reflection spectrum are thought to be produced by K-shell photoionization due to an external hard X-ray source which irradiates the accretion disk (such as synchrotron radiation from the relativistic jets emitted at the poles of the black holes, or radiation produced by flares in the disk and accelerated in the disk corona), the K-threshold lowering should have some effects on the K-line emissivities. Moreover, it may also provoke changes in the disk opacity. Actually, due to the radial distribution of the electron density in the disk, the so-called K-edge (the abrupt jump in the opacity caused by the absorption around the K-threshold energy) should appear broadened by the superposed K-thresholds that are shifted in different magnitudes depending on the local electron density. The corrections due to plasma environment effects for the ionization potentials and K-thresholds of all the oxygen ions should thus be introduced in the astrophysical simulation codes for modeling the reflection spectrum of an accreting black hole in a more precise way.

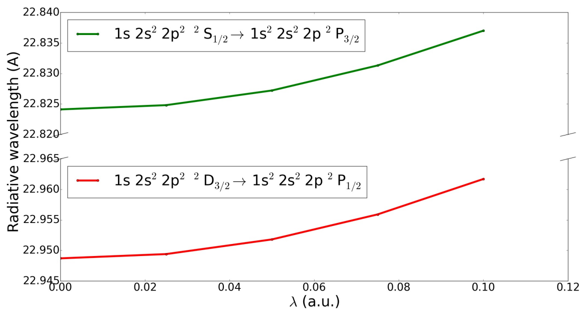

Figure 2: *Variation of the wavelengths with the plasma screening parameter λ for two K-lines in O IV (computed by MCDF/RATIP)*

Conclusion and perspectives

Our work, briefly presented in this paper, consists in the study of plasma environment effects on the atomic processes involved in the formation of K-lines in astrophysically important ions. These lines are of paramount interest for investigating the physical conditions of plasmas such as those observed in accretion disks around black holes, where electronic temperature ranging from 10^5 to 10^7 K and electronic density ranging from 10^{18} to 10^{21} cm^{-3} can be

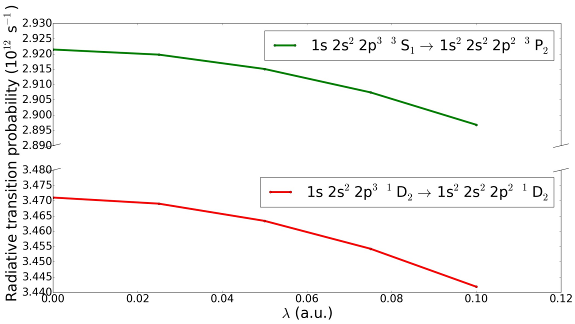

Figure 3: *Variation of the transition probabilities with the plasma screening parameter λ for two K-lines in O III (computed by MCDF/RATIP)*

expected, as well as for inferring some properties of the black hole itself. In the computational procedure, the plasma effects are modeled by means of a Debye-Hückel potential including the screening on both the electron-nucleus and electron-electron electrostatic interactions in the framework of two independent theoretical approaches, *i.e.* the multiconfiguration Dirac-Fock and the AUTOSTRUCTURE methods. From the results obtained, in the case of oxygen ions, we note that, for typical physical conditions in accretion disks around black holes, the ionization potentials as well as the K-thersholds are lowered by several eV compared to the isolated ion case, whereas K-lines are all redshifted by at most 10^{-2} Å and radiative transition probabilities are slightly reduced, namely by 1% on average. Hence, there is no need to modify the K-line radiative parameters used in the astrophysical simulation codes for that type of conditions, whereas corrections due to plasma environment should be incorporated for the ionization potentials and K-thresholds of all the oxygen ions in order to model the accretion disk reflection spectra at best. In the near future, we are planning to investigate the plasma environment effects on the atomic structure and radiative parameters for other cosmologically abundant ions, such as iron ions. The study of plasma effects on non-radiative parameters involved in the K-line formation, such as Auger rates, photoionization cross-sections and recombination rates is also foreseen but the atomic codes still need to be modified for that purpose.

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