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ATOMIC DATA CALCULATIONS FOR FE II AND CA II

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RESUMEN

Nosotros presentamos los cálculos para el Ca II y Fe II con el código AUTOSTRUCTURE. Para obtener el cálculo de dichas estructuras atómicas, se modificó el funcional que resulta del método variacional con el fin de mejorar los resultados que involucran configuraciones tales como $5l$ y $6l$. Por otro lado, también se modificó el método de optimización de los parámetros variacionales del código, específicamente por una subrutina del Gradiente Conjugado con el fin de encontrar una mejor y más rápida convergencia del modelo.

ABSTRACT

We presents calculations for Ca II and Fe II with the atomic structure AUTOSTRUTURE code. We introduced an improved functional in the variational optimization in order to enhance the results from configurations that include $5l$ and $6l$ orbitals. We have changed the minimization method of the variational parameters, specifically in subroutine Conjugated Gradient, in order to automate the minimization of the parameters and to speed convergence.

Key Words: atomic data

1. GENERAL

The spectra, ionization structure, and abundance of iron are valuable indicators of the physical conditions and chemical evolution of astrophysical objects. First, owing to the relatively high abundance of iron and the complex atomic structure of Fe Ions, a large number of spectral lines are observed across most of the electromagnetic spectrum. Second, several ionization stages of iron may be observed from diferent zones within the same object (Bautista & Pradhan 1998).

Ca II plays a prominent role in astrophysics. The so-called H and K lines of this ion are important probes of solar and stellar chromospheres (Rauscher & Marcy 2006). In the red spectra of Active Galactic Nuclei (AGN) the infrared triplet of Ca II in emission has been used to investigate the correlations with optical Fe II and their implications on the physical conditions of the emitting gas. [Ca II] optical emission lines together with the infrared [Fe II] are often used as probe of dust content of AGNs (Shields et al. 1999).

A more detailed study about Ca II and Fe II, that provides a better and more complete data base of the energy levels and transition probability, gives the adecuate information in order to a better comprehension of these astrophycal objects.

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2. ATOMIC DATA

2.1. *Atomic structure calculations*

We use the atomic structure code AUTOSTRUCTURE (Badnell 1986, 1997) to reproduce the structure of the Ca II and Fe II ion. This code is based on the program SUPERSTRUCTURE originally developed by (Eissner et al. 1974) but incorporates various improvements and new capabilities like two-body non-fine-structure operators of the Breit-Pauli Hamiltonian and polarization model potentials. In this approach, the wavefunctions are written as configuration interaction expansions of the type:

$$\Psi_i = \sum_j c_{ij}\phi_j \,, \tag{1}$$

where the coefficients c_{ij} are determined by diagonalization of $\langle \Psi_i | H | \Psi_j \rangle$. Here H is the Hamiltonian and the basic functions ϕ_j are constructed from one-electron orbitals generated using the Thomas-Fermi-Dirac model potential (Eissner & Nussbaumer 1969), including λ_{nl} scaling parameters which are optimized by minimizing a weighted sum of energies, implementated the variational method:

$$E_i = E_i(\lambda_{nl}) = \langle \Psi_i | H_{nr} | \Psi_j \rangle \,, \tag{2}$$

where H_{nr} is the usual non-relativistic Hamiltonian. Now can to define the F functional as:

$$\delta F = \delta \left\{ \sum_{i=1}^{NE} g_i E_i(\lambda_{nl}) \right\} = 0, \tag{3}$$

where NE is the energy number included in the minimization process.

Relativistic effects are included in the calculation by means of the Breit-Pauli operators in the form:

$$H = H_{nr} + H_{bp}, \qquad (4)$$

where H_{bp} is the Breit-Pauli perturbation, which indudes one- and two-body operators (Jones 1970).

2.2. *A new functional*

We introduce a new functional form by the percentage diferences between the observed energies from NIST and energy calculated using AUTOSTRUCTURE code.

$$\delta F = \delta \sum_{i=1}^{NE} g_i \left[\frac{|E_i^{\rm obs} - E_i(\lambda_{nl})| + \varepsilon}{E_i^{obs}} \right]^2 = 0 \qquad (5)$$

where $E_i^{\rm obs}$ is the observational energy from NIST and ε is the core energy.

2.3. *Conjugated Gradient*

The orbitals are very close to the continuum so there is strong overlap between them, being difficult to determine the energy levels because the variational method presents problems minimizing a large number of terms. We have changed the minimization method of the variational parameters of AUTOSTRUCTURE, which originaly had a Powell method for a Conjugated Gradient method, in order to automate the minimization of the parameters and to speed convergence.

3. RESULTS

The results of the present calculations include the following sets of data: (a) the comparison between differents methods implemented by Ca II and (b) the comparison between different methods implemented by Fe II.

3.1. *Energy levels*

The results of Ca II contain the next configurations: $3d$, $4s$, $4d$, $4p$, $4f$, $5s$, $5p$, $5d$, $5f$, $5g$, $6s$, $6p$, $6d$, $6f$, $6g$, $7s$, $7d$, $7f$, $7g$, $8s$, $8d$, $8f$, $8g$, and of Fe II contain 16-configuration expansion, including $3d^7$, $3d^6 4s$, $3d^6 4p$ (Bautista & Pradhan 1997) and new 36-configuration with $4d$, $4f$, $5s$, $5p$, $5d$, $6s$ and $6p$. Figures 1 and 2 show (A) the calculations using the original AUTOSTRUCTURE code, (B) the calculations using AUTOSTRUCTURE code with the new funtional and (C) calculations using AUTOSTRUCTURE code with, Conjugated Gradient method.

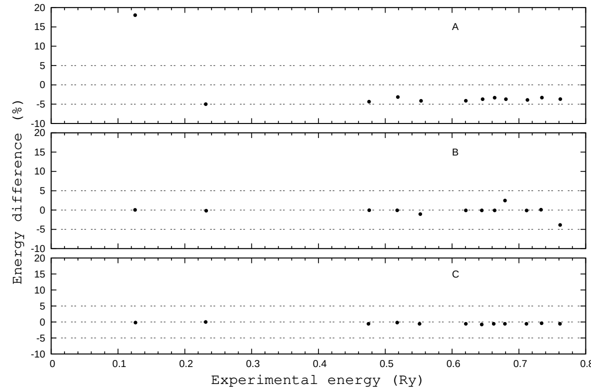

Fig. 1. Calculation for ion Ca II.

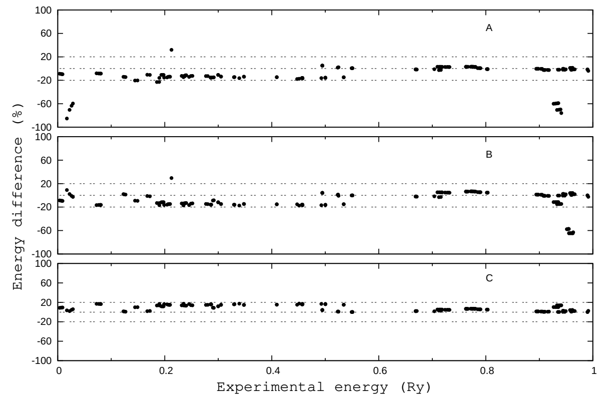

Fig. 2. Calculation for ion Fe II.

4. DISCUSSION AND CONCLUSION

We have computed energy levels for Ca II and Fe II using AUTOSTRUCTURE code. Here we found that the results obtained with Conjugated Gradient are the best, both for Ca II as for Fe II.

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