LAGUERRE POLYNOMIALS IN A RELATIVISTIC QUANTUM-STATISTICAL MODEL.

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Abstract

The main aim of this work is to find analytical expressions for the eigenvalues and eigenfunctions corresponding to Dirac equation, for hot and dense matter. It is shown that the Laguerre polynomials depending on the effective charge are solutions for self-consistent fields. To determine the screening constant and effective charge we introduce and minimize a functional. These formulas are accurate for machine calculation of bound-bound, bound-free and free-free transitions, including large values of principal quantum numbers. Hence these expressions would be in accordance with quantum-statistical results based on more sophisticated calculations. Comparisons with the solutions of the Schrödinger equation for different substancies are disscused.

1 Introduction.

The Knowledge of the wave functions plays a fundamental role in quantum physics, e.g., quantum-statistical models, such as opacity and equation of state calculations [1], [4], [6], [7] and [11].
When one comes to compute the wave functions and energy levels, two methods are usually employed. The first one, which involves sophisticated calculations, consists in solving the Schrödinger or Dirac equation. This is very expensive because the model requires very long computational time, mainly when is necessary to take into account the multiconfigurability of the heavy atoms, then the use of supercomputers is justified. The second one is based on approximate expressions. In light of this development we propose in the present work a simple and fast model, which doesn't require to solve the Dirac or Schrödinger equation, and determines, by means of an analytical expression, the wave functions and energy levels for each electron of high-Z elements at high temperatures and densities, mainly in the cases, where the computational time can be very long. This model has been developed as kernel of future code for opacity calculations and other physical applications.
The structure of paper is as follows. In Section 2 we provide the required background about the solutions of the Dirac equation via Laguerre polynomials, giving analytical expressions for wave functions and energy levels, depending on the effective charge and screening constant. In Section 3, we define a functional, depending on the effective charge and screening constant. Hence we describe the minimization procedure of this functional. The found extremum allows us to obtain the wave functions and energy levels, since it depends on the effective charge and screening constant. This method is proposed to avoid solving the Dirac equation numerically, and so that, we can save a considerable amount of computer memory part. This method is being compared with other one [12]. Finally, in Section 4 we provide a table of numerical results and some graphics and compare them with results from other methods, in order to determine the accuracy of our approximation.

2 The wave function dependence on effective charge.

The wave functions corresponding to the numerical solution of the Dirac equation for a self-consistent field in high temperature plasmas at high-Z elements, have hydrogenic behaviour.

From this behaviour of the wave function suitable to electrons with any combination of quantum numbers nlj, and from their similarity with Laguerre functions, the idea of a generalized representation of Hartree, conserving the spherical symmetry has arised. In this representation the quantum number j has been added.
In our approach each atomic electron moves in the individual potential $\widetilde{U}(r) = -\frac{Z_{nlj}}{r} + A_{nlj}$, depending on the nuclear charge and the other atomic electrons. Here we represent by Z_{nlj} the effective charge and by A_{nlj} the screening constant. Although, this assumption is an approximate description for the real hot and dense matter. However, it makes possible to understand the behavior of atoms and to find their energy levels and wave functions in a very simple way, because it constitutes a very difficult quantum mechanical many-body-problem. For the above potential we can solve, analytically, the Dirac equation. Therefore the wave functions are expressed in analytical form, depending on Z_{nlj} this guarantees to operate with them easily. Thus the efforts shall reduce in order to find the appropriate values of the effective charge Z_{nlj} and screening constant A_{nlj}, respectively.
Before proceeding with a description of the method, it is useful to explain which physical approximations will be assumed
1. With a good degree of accuracy the atomic nuclei with respect to the atomic electrons can be consider fixed strenght centers.
2. The electrons are continuosly distributed in the phase space according to Fermi-Dirac statistics.
3. The existence in the atomic nuclei of electric quadrupole, magnetic dipole and all higher multipole orders are neglected.
The reason for which more work is dedicated to the attainment of the most exactly possible wave functions (and not justly in the attainment of the energy levels though both are closely linked by means of the Dirac equation) is conditioned for the calculations of radiative transition probabilities bound-bound, bound-free and free-free to be incorporated into opacity calculation. For the purpose of getting a better quantitative understanding of the dependence of the radial wave function on the Z_{nlj} and A_{nlj}, we summarize here the essential points in the procedure to obtain it in a most adequate form. First, we must obtain the exact solution of the Dirac differential equation for an electron in a potential $\widetilde{U}(r) = -\frac{Z_{nlj}}{r} + A_{nlj}$, for stationary states with discrete spectra of total energy $\widetilde{E}$ it is given by [3]

$$\widetilde{\hat{H}}\widetilde{\Psi} = \left[c(\vec{\alpha}\vec{\hat{p}}) + mc^2\beta + \widetilde{U}(r)\right]\widetilde{\Psi} = \widetilde{E}\widetilde{\Psi},$$

where $\widetilde{\Psi}$ is a 1 column-4 row matrix, i.e., the spinor of four components

$$\widetilde{\Psi} = \begin{pmatrix} \widetilde{\psi}_1 \\ \widetilde{\psi}_2 \\ \widetilde{\psi}_3 \\ \widetilde{\psi}_4 \end{pmatrix}, \quad (\vec{\alpha}\vec{\hat{p}}) = \sum_{k=1}^{3} \alpha_k \hat{p}_k, \quad \left(\hat{p}_k = \frac{\hbar}{i}\frac{\partial}{\partial x_k}\right), \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix},$$

being the components of σ_k and β the following two-by-two matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \text{and} \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad 0 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

The symbols with tilde are used in this work to distinguish both the hydrogenic-like magnitudes and wave functions from those wave functions corresponding to the exact solution of the Dirac equation for the hydrogen.
Writing explicitly the Dirac equation for the four components of the wave function, taking into account relativistic units, i.e., the mass of the electron, Planck's constant $\hbar$, and the speed of light

are all equal to 1, it holds

$$
\begin{aligned}
&i\left(\widetilde{\varepsilon}+\frac{\widetilde{\mu}}{r}+1\right)\widetilde{\psi}_1+\frac{\partial\widetilde{\psi}_3}{\partial z}+\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)\widetilde{\psi}_4=0,\\
&i\left(\widetilde{\varepsilon}+\frac{\widetilde{\mu}}{r}+1\right)\widetilde{\psi}_2-\frac{\partial\widetilde{\psi}_4}{\partial z}+\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)\widetilde{\psi}_3=0,\\
&i\left(\widetilde{\varepsilon}+\frac{\widetilde{\mu}}{r}-1\right)\widetilde{\psi}_3+\frac{\partial\widetilde{\psi}_1}{\partial z}+\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)\widetilde{\psi}_2=0,\\
&i\left(\widetilde{\varepsilon}+\frac{\widetilde{\mu}}{r}-1\right)\widetilde{\psi}_4-\frac{\partial\widetilde{\psi}_2}{\partial z}+\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)\widetilde{\psi}_1=0,
\end{aligned}
\tag{1}
$$

where

$$
\widetilde{\mu}=\widetilde{\mu}_{nlj}=\frac{Z_{nlj}e^2}{\hbar c}\approx\frac{Z_{nlj}}{137},\quad \widetilde{E}_{nlj}=\widetilde{\varepsilon}+A_{nlj},\quad (0<\widetilde{E}_{nlj}<1)\quad .
$$

In spherical coordinates $(r,\ \theta,\ \varphi)$ the variables in these equations can be separated –if one makes use of the fact that the components and the absolute value of the total angular momentum of an electron in any central force field are constants of the motion, then we can construct the eigenfunction of the eigenvalues which correspond to operators $\hat{H},\ \hat{J}^2$ and $\hat{J}_Z$, i.e, we base on the spherical symmetry the field of the nucleus– by looking for a solution that has the form [9], [10]

$$
\begin{pmatrix}\widetilde{\psi}_1\\ \widetilde{\psi}_2\end{pmatrix}=\widetilde{f}_{nlj}(r)\Theta_{nlm}(\theta,\varphi),\qquad \begin{pmatrix}\widetilde{\psi}_3\\ \widetilde{\psi}_4\end{pmatrix}=(-1)^{(l-l'+1)/2}\widetilde{g}_{nlj}(r)\Theta_{nl'm}(\theta,\varphi),
$$

whence

$$
\begin{aligned}
&\widetilde{\Psi}=\begin{pmatrix}\widetilde{\psi}_1\\ \widetilde{\psi}_2\\ \widetilde{\psi}_3\\ \widetilde{\psi}_4\end{pmatrix}=(-1)^{\left(m-\frac{1}{2}\right)}i^l\begin{pmatrix}\sqrt{\frac{j+m}{2l+1}} & \widetilde{f}_{nlj}(r) & \Theta_{l,m-\frac{1}{2}}(\theta,\varphi)\\ -\sqrt{\frac{j-m}{2l+1}} & \widetilde{f}_{nlj}(r) & \Theta_{l,m+\frac{1}{2}}(\theta,\varphi)\\ -\sqrt{\frac{j-m+1}{2l+3}} & i\widetilde{g}_{nlj}(r) & \Theta_{l+1,m-\frac{1}{2}}(\theta,\varphi)\\ -\sqrt{\frac{j+m+1}{2l+3}} & i\widetilde{g}_{nlj}(r) & \Theta_{l+1,m+\frac{1}{2}}(\theta,\varphi)\end{pmatrix}\quad\text{for}\quad l=j-\tfrac{1}{2},\\
&\widetilde{\Psi}=\begin{pmatrix}\widetilde{\psi}_1\\ \widetilde{\psi}_2\\ \widetilde{\psi}_3\\ \widetilde{\psi}_4\end{pmatrix}=(-1)^{\left(m+\frac{1}{2}\right)}i^l\begin{pmatrix}\sqrt{\frac{j-m+1}{2l+1}} & \widetilde{f}_{nlj}(r) & \Theta_{l,m-\frac{1}{2}}(\theta,\varphi)\\ \sqrt{\frac{j+m+1}{2l+1}} & \widetilde{f}_{nlj}(r) & \Theta_{l,m+\frac{1}{2}}(\theta,\varphi)\\ \sqrt{\frac{j+m}{2l-1}} & i\widetilde{g}_{nlj}(r) & \Theta_{l-1,m-\frac{1}{2}}(\theta,\varphi)\\ -\sqrt{\frac{j-m}{2l-1}} & i\widetilde{g}_{nlj}(r) & \Theta_{l-1,m+\frac{1}{2}}(\theta,\varphi)\end{pmatrix}\quad\text{for}\quad l=j+\tfrac{1}{2}.
\end{aligned}
\tag{2}
$$

By substituting the explicit formulas (2) in (1) one then obtains [10]

$$
\begin{cases}
\widetilde{f}'_{nlj}+\frac{1+\kappa}{r}\widetilde{f}_{nlj}-\left(\widetilde{\varepsilon}_{nlj}+1+\frac{\widetilde{\mu}_{nlj}}{r}\right)\widetilde{g}_{nlj}=0,\\
\widetilde{g}'_{nlj}+\frac{1-\kappa}{r}\widetilde{g}_{nlj}-\left(\widetilde{\varepsilon}_{nlj}-1+\frac{\widetilde{\mu}_{nlj}}{r}\right)\widetilde{f}_{nlj}=0,
\end{cases}
\tag{3}
$$

where

$$
\kappa=\begin{cases}-(l+1) & \text{if}\quad l=j-\frac{1}{2},\\ l & \text{if}\quad l=j+\frac{1}{2}.\end{cases}\qquad l=0,1,...,n-1\quad .
$$

For bound states the wave functions $\widetilde{f}_{nlj}(r)$ and $\widetilde{g}_{nlj}(r)$ should satisfy the normalization condition

$$
\int_0^\infty\left[\widetilde{f}^2_{nlj}(r)+\widetilde{g}^2_{nlj}(r)\right]r^2\,dr=1,\quad\text{since}\quad \int_0^\pi\int_0^{2\pi}\left|\Theta_{l,m}(\theta,\varphi)\right|^2\,d\theta d\varphi=1.
\tag{4}
$$

The system (3) can be written in matrix form

$$\begin{pmatrix} \widetilde{f}'_{nlj}(r) \\ \widetilde{g}'_{nlj}(r) \end{pmatrix} = \mathbb{K}\cdot \begin{pmatrix} \widetilde{f}_{nlj}(r) \\ \widetilde{g}_{nlj}(r) \end{pmatrix}, \quad \text{where} \quad \mathbb{K} = \begin{pmatrix} -\dfrac{1+k}{r} & 1+\widetilde{\varepsilon}+\dfrac{\widetilde{\mu}}{r} \\ 1-\widetilde{\varepsilon}-\dfrac{\widetilde{\mu}}{r} & -\dfrac{1-k}{r} \end{pmatrix}. \tag{5}$$

This leads to the following system of second order differential equations

$$\begin{aligned} &\widetilde{f}''_{nlj}(r) - \tau_1(r)\widetilde{f}'_{nlj}(r) + \lambda_1(r)\widetilde{f}_{nlj}(r) = 0, \\ &\widetilde{g}''_{nlj}(r) - \tau_2(r)\widetilde{g}'_{nlj}(r) + \lambda_2(r)\widetilde{g}_{nlj}(r) = 0, \end{aligned} \tag{6}$$

where

$$\begin{aligned} \tau_1(r) &= -\left[\tfrac{2}{r} + \tfrac{\widetilde{\mu}}{r^2(1+\widetilde{\varepsilon})+r\widetilde{\mu}}\right],\ \lambda_1(r) = \tfrac{1-k^2}{r} - \left[1-(\widetilde{\varepsilon}+\tfrac{\widetilde{\mu}}{r})^2\right] - \tfrac{1+k}{r^2} + \tfrac{\widetilde{\mu}(1+k)}{r^3(1+\widetilde{\varepsilon})+r^2\widetilde{\mu}}, \\ \tau_2(r) &= -\left[\tfrac{2}{r} - \tfrac{\widetilde{\mu}}{r^2(1-\widetilde{\varepsilon})-r\widetilde{\mu}}\right],\ \lambda_2(r) = \tfrac{1-k^2}{r} - \left[1-(\widetilde{\varepsilon}+\tfrac{\widetilde{\mu}}{r})^2\right] - \tfrac{1-k}{r^2} - \tfrac{\widetilde{\mu}(1-k)}{r^3(1+\widetilde{\varepsilon})+r^2\widetilde{\mu}}. \end{aligned} \tag{7}$$

The equations (6) are not generalized equations of hypergeometric type, since $1+\widetilde{\varepsilon}\neq 0$ and $\widetilde{\mu}\neq 0$. By means of a linear transformation the system (6) becomes in a similar one, which under certain conditions can be transformed in a generalized system of equations of hypergeometric type. Let be the system

$$\mathbb{L}\cdot \begin{pmatrix} \widetilde{f}_{nlj}(r) \\ \widetilde{g}_{nlj}(r) \end{pmatrix} = \widetilde{\mathsf{Y}} = \begin{pmatrix} \widetilde{y}_1 \\ \widetilde{y}_2 \end{pmatrix},$$

where $\mathbb{L}$ is a nonsingular matrix independent of r. Therefore

$$\widetilde{\mathsf{Y}}' = \begin{pmatrix} \widetilde{y}'_1 \\ \widetilde{y}'_2 \end{pmatrix} = \widetilde{\mathbb{K}}\cdot\widetilde{\mathsf{Y}},\ \text{where}\ \widetilde{\mathbb{K}} = \mathbb{L}\cdot\mathbb{K}\cdot\mathbb{L}^{-1} = \begin{pmatrix} \widetilde{k}_{11} & \widetilde{k}_{12} \\ \widetilde{k}_{21} & \widetilde{k}_{22} \end{pmatrix},\ \text{and}\ \mathbb{L} = \begin{pmatrix} \widetilde{l}_{11} & \widetilde{l}_{12} \\ \widetilde{l}_{21} & \widetilde{l}_{22} \end{pmatrix}. \tag{8}$$

The elements of $\widetilde{\mathbb{K}}$ are

$$\begin{aligned} \widetilde{k}_{11} &= (\det\mathbb{L})^{-1}\left[-\frac{1+k}{r}l_{11}l_{22} - (1+\widetilde{\varepsilon}+\frac{\widetilde{\mu}}{r})l_{11}l_{21} + (1-\widetilde{\varepsilon}-\frac{\widetilde{\mu}}{r})l_{12}l_{22} + \frac{1-k}{r}l_{12}l_{21}\right], \\ \widetilde{k}_{12} &= (\det\mathbb{L})^{-1}\left[(1+\widetilde{\varepsilon}+\frac{\widetilde{\mu}}{r})l_{11}^2 - (1-\widetilde{\varepsilon}-\frac{\widetilde{\mu}}{r})l_{12}^2 + \frac{2k}{r}l_{11}l_{12}\right], \\ \widetilde{k}_{21} &= (\det\mathbb{L})^{-1}\left[(1-\widetilde{\varepsilon}-\frac{\widetilde{\mu}}{r})l_{22}^2 - (1+\widetilde{\varepsilon}+\frac{\widetilde{\mu}}{r})l_{21}^2 - \frac{2k}{r}l_{21}l_{22}\right], \\ \widetilde{k}_{22} &= (\det\mathbb{L})^{-1}\left[\frac{1+k}{r}l_{12}l_{21} + (1+\widetilde{\varepsilon}+\frac{\widetilde{\mu}}{r})l_{11}l_{21} - (1-\widetilde{\varepsilon}-\frac{\widetilde{\mu}}{r})l_{12}l_{22} - \frac{1-k}{r}l_{11}l_{22}\right]. \end{aligned} \tag{9}$$

From the equations for $\widetilde{y}_1(r)$ and $\widetilde{y}_2(r)$ we get

$$\widetilde{y}''_1(r) - \widetilde{\tau}_1(r)\widetilde{y}'_1(r) + \widetilde{\lambda}_1(r)\widetilde{y}_1(r) = 0, \tag{10}$$

$$\widetilde{y}''_2(r) - \widetilde{\tau}_2(r)\widetilde{y}'_2(r) + \widetilde{\lambda}_2(r)\widetilde{y}_2(r) = 0, \tag{11}$$

where

$$\begin{aligned} \widetilde{\tau}_1(r) &= \left(\widetilde{k}_{11} + \widetilde{k}_{22} + \frac{\widetilde{k}'_{12}}{\widetilde{k}_{12}}\right), \quad \widetilde{\lambda}_1(r) = \left(\widetilde{k}_{11}\widetilde{k}_{22} - \widetilde{k}_{12}\widetilde{k}_{21} - \widetilde{k}'_{11} + \frac{\widetilde{k}'_{12}}{\widetilde{k}_{12}}\widetilde{k}_{11}\right), \\ \widetilde{\tau}_2(r) &= \left(\widetilde{k}_{11} + \widetilde{k}_{22} + \frac{\widetilde{k}'_{21}}{\widetilde{k}_{21}}\right), \quad \widetilde{\lambda}_1(r) = \left(\widetilde{k}_{11}\widetilde{k}_{22} - \widetilde{k}_{12}\widetilde{k}_{21} - \widetilde{k}'_{22} + \frac{\widetilde{k}'_{21}}{\widetilde{k}_{21}}\widetilde{k}_{22}\right). \end{aligned} \tag{12}$$

The equations (10) and (11) become into equations of generalized hypergeometric type if we impose the conditions

$$2kl_{11}l_{12} + \widetilde{\mu}(l_{12}^2 + l_{12}^2) = 0 \quad \text{and} \quad 2kl_{21}l_{22} + \widetilde{\mu}(l_{21}^2 + l_{22}^2) = 0.$$

Notice that we select two among four possibilities to transform (10) and (11) into equations of generalized hypergeometric type. Then, $\mathbb{L}$ takes the form

$$\mathbb{L} = \begin{pmatrix} \widetilde{\mu} & \widetilde{\nu} - k \\ \widetilde{\nu} - k & \widetilde{\mu} \end{pmatrix}, \text{ where } \widetilde{\nu} = \sqrt{\kappa^2 - \widetilde{\mu}^2}. \tag{13}$$

In the case when $1 + \frac{\varepsilon\kappa}{\widetilde{\nu}} \neq 0$, we obtain the following differential equation for $\widetilde{y}_1(r)$

$$\widetilde{y}_1''(r) + \frac{2}{r}\widetilde{y}_1'(r) + \frac{(\widetilde{\varepsilon}^2 - 1)r^2 + 2\widetilde{\varepsilon}\mu r - \widetilde{\nu}(\widetilde{\nu} + 1)}{r^2}\widetilde{y}_1(r) = 0. \tag{14}$$

In the opposite cases $1 + \frac{\varepsilon\kappa}{\widetilde{\nu}} = 0$, then we deduce that that $\widetilde{y}_1(r) = 0$ and $\widetilde{y}_2(r) = 0$. This kind of functions don't satisfy (4). In order to determine the behavior of $\widetilde{y}_1(r)$ in the neighborhood of $r = 0$ we require

$$|(\widetilde{\varepsilon}^2 - 1)r^2 + 2\widetilde{\varepsilon}\widetilde{\mu}r| \ll \widetilde{\nu}(\widetilde{\nu} + 1),$$

and then $\widetilde{y}_1(r) \approx C_1 r^{\widetilde{\nu}}$ for small enough r.

Equation (14) is a generalized equation of hypergeometric type. In order to (14) will be an equation of hypergeometric type

$$\sigma(r)y'' + \tau(r)y' + \lambda y = 0,$$

where, $\sigma(r)$ and $\tau(r)$ are polynomials of degree at most 2 and 1, respectively; we substitute $\widetilde{y}_1$ by $\phi(r)y$, where $\phi(r)$ satisfies

$$\phi'/\phi = \pi(r)/\sigma(r).$$

We choose $\tau(r) = \widetilde{\tau}(r) + 2\pi(r)$ with negative derivative and zero on $(0,+\infty)$. These conditions impose restrictions on the choice of $\pi(r)$, hence we get $\pi(r) = -\widetilde{a}r + \widetilde{\nu}$, with $\widetilde{a} = \sqrt{1 - \widetilde{\varepsilon}^2}$. Whence

$$\sigma(r) = r, \quad \tau(r) = 2(\widetilde{\nu} + 1 - \widetilde{a}r), \quad \phi(r) = r^{\widetilde{\nu}}e^{-\widetilde{a}r}, \quad \lambda = 2[\widetilde{\varepsilon}\widetilde{\mu} - (\widetilde{\nu} + 1)\widetilde{a}], \quad \rho(r) = r^{2\widetilde{\nu}+1}e^{-2\widetilde{a}r}.$$

The eigenvalues are determined by [10]

$$\lambda + n\tau' + \frac{1}{2}n(n-1)\sigma'' = 0, \quad n = 0, 1, 2, ...$$

and the eigenfunctions follow from the Rodrigues formula [10]

$$y_n(r) = \frac{C_n}{\rho(r)}\frac{d^n}{dr^n}[\sigma^n(r)\rho(r)] = C_n r^{-2\widetilde{\nu}-1}e^{2\widetilde{a}r}\frac{d^n}{dr^n}(r^{n+2\widetilde{\nu}+1}e^{-2\widetilde{a}r}). \tag{15}$$

The functions $y_n(r)$ are, up to a constant factor, the Laguerre polynomials $L_n^{2\widetilde{\nu}+1}(x)$, with $x = 2\widetilde{a}r$. In order to obtain the equivalence with quantum mechanic interpretation we replace n by $n - 1$, then

$$\widetilde{\mu}\widetilde{\varepsilon} - (n + \widetilde{\nu} + 1)\widetilde{a} = 0. \tag{16}$$

As a consequence the eigenfuctions $\widetilde{y}_1(r)$ take the form

$$\widetilde{y}_1(r) = \begin{cases} A_n x^{\widetilde{\nu}} e^{-x/2} L_{n-1}^{2\widetilde{\nu}+1}(x) & n=1,2,..., \\ 0 & n=0. \end{cases} \tag{17}$$

Using (11), (16) and (17) we find a similar differential equation for $\widetilde{y}_2$

$$\widetilde{y}_2''(r) + \frac{2}{r}\widetilde{y}_2' + \frac{(\widetilde{\varepsilon}^2 - 1)r^2 + 2\widetilde{\varepsilon}\mu r + \widetilde{\nu}(\widetilde{\nu} - 1)}{r^2}\widetilde{y}_2 = 0. \tag{18}$$

From (18) it follows that the eigenfunctions are

$$\widetilde{y}_2(r) = B_n x^{\widetilde{\nu}-1} e^{-x/2} L_n^{2\widetilde{\nu}-1}(x). \tag{19}$$

Using (8), (9) and (13) we find

$$\widetilde{y}_1' = \left(-\frac{\widetilde{\nu}+1}{r} + \frac{\widetilde{\varepsilon}\kappa}{\widetilde{\nu}}\right)\widetilde{y}_1 + \left(1 + \frac{\widetilde{\varepsilon}\kappa}{\widetilde{\nu}}\right)\widetilde{y}_2, \tag{20}$$

putting the explicit formula for $\widetilde{y}_1$ as well as $r = 0$ in (20) and taking into account that [10]

$$L_n^\alpha(0) = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)}.$$

We have

$$A_n = \frac{\widetilde{\nu} + \widetilde{\varepsilon}\kappa}{\widetilde{a}n(n+2\widetilde{\nu})}B_n \qquad (n = 1, 2, ...).$$

Since we know $\widetilde{y}_1(r)$ and $\widetilde{y}_2(r)$, we can give the analytic expression for the radial components of the wave functions $\widetilde{f}_{nlj}(r)$ and $\widetilde{g}_{nlj}(r)$

$$\begin{pmatrix} \widetilde{f}_{nlj} \\ \widetilde{g}_{nlj} \end{pmatrix} = \frac{1}{2\widetilde{\nu}(\kappa - \widetilde{\nu})} \begin{pmatrix} \widetilde{\mu} & \widetilde{\nu} - \kappa \\ \widetilde{\nu} - \kappa & \widetilde{\mu} \end{pmatrix} \cdot \begin{pmatrix} \widetilde{y}_1 \\ \widetilde{y}_2 \end{pmatrix}, \tag{21}$$

from which

$$\begin{aligned} \widetilde{f}_{nlj}(r)\Big|_{r=\frac{x}{2\widetilde{a}}} &= \frac{B_n}{2\widetilde{\nu}(\kappa - \widetilde{\nu})} x^{\widetilde{\nu}-1} e^{-\frac{x}{2}} \left(f_1 x L_{n-1}^{2\widetilde{\nu}+1}(x) + f_2 L_n^{2\widetilde{\nu}-1}(x)\right), \\ \widetilde{g}_{nlj}(r)\Big|_{r=\frac{x}{2\widetilde{a}}} &= \frac{B_n}{2\widetilde{\nu}(\kappa - \widetilde{\nu})} x^{\widetilde{\nu}-1} e^{-\frac{x}{2}} \left(g_1 x L_{n-1}^{2\widetilde{\nu}+1}(x) + g_2 L_n^{2\widetilde{\nu}-1}(x)\right), \end{aligned} \tag{22}$$

where

$$B_n = 2\widetilde{a}\sqrt{\frac{(\kappa - \widetilde{\nu})(\widetilde{\varepsilon}\kappa - \widetilde{\nu})n!}{\widetilde{\mu}\Gamma(n+2\widetilde{\nu})}}, \quad \widetilde{\varepsilon} = \frac{1}{\sqrt{1 + \left(\frac{\widetilde{\mu}}{n+\widetilde{\nu}}\right)^2}}, \quad \widetilde{\nu} = \sqrt{(j+\frac{1}{2})^2 - \widetilde{\mu}^2},$$

$$\widetilde{a} = \frac{\frac{\widetilde{\mu}}{n+\widetilde{\nu}}}{\sqrt{1+\left(\frac{\widetilde{\mu}}{n+\widetilde{\nu}}\right)^2}}, \quad f_1 = \frac{\widetilde{a}\widetilde{\mu}}{\widetilde{\varepsilon}\kappa - \widetilde{\nu}}, \quad f_2 = \kappa - \widetilde{\nu}, \quad g_1 = \frac{\widetilde{a}(\kappa - \widetilde{\nu})}{\widetilde{\varepsilon}\kappa - \widetilde{\nu}}, \quad g_2 = \widetilde{\mu}.$$

To calculate B_n we have used the orthonormality condition, the three-term recurrence relation and the following expansion formula for the Laguerre polynomials [10]

$$L_n^{\alpha-2}(x) = L_n^\alpha(x) - 2L_{n-1}^\alpha(x) + ...$$

The solutions (22) in atomic units take the form

$$\widetilde{F}_{nlj}(r)\Big|_{r=\frac{x}{137\cdot 2\widetilde{a}}} = r\widetilde{f}_{nlj}(r) = (137)^{\frac{1}{2}} \frac{\widetilde{B}_{nlj}}{4\widetilde{a}\widetilde{\nu}(\kappa - \widetilde{\nu})} x^{\widetilde{\nu}} e^{-\frac{x}{2}} \left(\widetilde{f}_1 x L_{n-j-\frac{3}{2}}^{2\widetilde{\nu}+1}(x) + \widetilde{f}_2 L_{n-j-\frac{1}{2}}^{2\widetilde{\nu}-1}(x)\right),$$

$$\widetilde{G}_{nlj}(r)\Big|_{r=\frac{x}{137\cdot 2\widetilde{a}}} = r\widetilde{g}_{nlj}(r) = (137)^{\frac{1}{2}}\frac{\widetilde{B}_{nlj}}{4\widetilde{a}\widetilde{\nu}(\kappa-\widetilde{\nu})}x^{\widetilde{\nu}}e^{-\frac{x}{2}}\left(\widetilde{g}_1 x L^{2\widetilde{\nu}+1}_{n-j-\frac{3}{2}}(x)+\widetilde{g}_2 L^{2\widetilde{\nu}-1}_{n-j-\frac{1}{2}}(x)\right),$$

$$\widetilde{B}_{nlj} = \frac{2\widetilde{a}^2}{\widetilde{\mu}}\sqrt{\frac{(\kappa-\widetilde{\nu})(n-j-\frac{1}{2})![\widetilde{a}\kappa(n-j-\frac{1}{2}+\widetilde{\nu})-\widetilde{\mu}\widetilde{\nu}]}{\Gamma(n-j-\frac{1}{2}+2\widetilde{\nu})}},\quad \widetilde{a} = \frac{\frac{\widetilde{\mu}}{n-j-\frac{1}{2}+\widetilde{\nu}}}{\sqrt{1+\left(\frac{\widetilde{\mu}}{n-j-\frac{1}{2}+\widetilde{\nu}}\right)^2}},$$

$$\widetilde{f}_1 = \frac{\widetilde{a}\widetilde{\mu}^2}{\widetilde{a}\kappa(n-j-\frac{1}{2}+\widetilde{\nu})-\widetilde{\mu}\widetilde{\nu}},\quad \widetilde{f}_2=\kappa-\widetilde{\nu},\quad \widetilde{g}_1=\frac{\kappa-\widetilde{\nu}}{\widetilde{\mu}}\widetilde{f}_1,\quad \widetilde{g}_2=\widetilde{\mu},$$

$$\widetilde{n} = n-\frac{\widetilde{\mu}^2}{(j+\frac{1}{2})+\sqrt{(j+\frac{1}{2})^2-\widetilde{\mu}^2}},\quad \widetilde{\varepsilon}_{nlj} = -\frac{\frac{Z^2}{\widetilde{n}^2}}{1+\frac{\widetilde{\mu}^2}{\widetilde{n}^2}+\sqrt{1+\frac{\widetilde{\mu}^2}{\widetilde{n}^2}}},\widetilde{\nu}=\sqrt{(j+\frac{1}{2})^2-\widetilde{\mu}^2},$$

$$n=1,2,\dots,\quad j=\frac{1}{2},\frac{3}{2},\dots,n-\frac{1}{2}\quad .$$

Notice that we have replaced $\widetilde{f}_{nlj}(r)$ and $\widetilde{g}_{nlj}(r)$ by $\widetilde{F}_{nlj}(r)$ and $\widetilde{G}_{nlj}(r)$, respectively to remark the difference between the wave function in relativistic units and the wave function in atomic units. From the above expressions it is clear that whether we are able to find the effective charge we can construct the atomic wave functions. In the next section we propose a simple method to determine it.

3 Calculation of the effective charge.

At this point it is important to construct and minimize a functional, whose dependence is given in terms of the variables Z_{nlj} and A_{nlj}, so the wave functions and energy levels can be expressed analytically for a self-consistent field [2]. This procedure constitutes an alternative method to avoid solving numerically the Dirac equation for each state at given potential.
When one solves a quantum-statistical problem we calculate the Thomas-Fermi potential $U_{T-F}(r)$ or the Hartree-Fock-Slater $U_{H-F-S}(r)$ one. Both potentials depend on the temperature (θ) and density (ρ). The product $rU(r)$ is approximated by a linear function on a restricted interval of r in which the absolute maximum or minimum of the wave function is located, i.e., in the region of r where the wave function certainly is different from zero (the most probable position for the particle). Let be take the following linear function,

$$F(r)\equiv Z_{nlj}-rA_{nlj} = -r\widetilde{U}(r),\quad r\in[0,+\infty[.$$

All this can be expressed mathematically by means of a functional $\Phi(Z_{nlj},A_{nlj})$,

$$\Phi(Z_{nlj},A_{nlj}) = \int_0^\infty\left[rU(r)-r\widetilde{U}(r,Z_{nlj},A_{nlj})\right]^2\left[\widetilde{F}^2_{nlj}(r)+\widetilde{G}^2_{nlj}(r)\right]dr. \qquad (23)$$

Whereby the radial components of the wave functions corresponding to the self-consistent field $U(r)$ will be almost equal to the radial components of the analytic wave functions $\widetilde{F}_{nlj}(r)$ and $\widetilde{G}_{nlj}(r)$ for the parametric potential $\widetilde{U}(r)$.
Notice that the behavior of the curve $rU(r)$ depends on the choice range of temperature and density. Although this model is applicable on the restricted range of temperature and density our numerical simulations shown that it cover a wide region of densities and temperatures: $10^{-3}g/cm^3\le\rho\le 10^2 g/cm^3$, $5ev\le\theta\le 15Kev$, depending on the substance and quantum number combinations.

Without a preliminary analysis the functional $\Phi(Z_{nlj}, A_{nlj})$, can be minimized under conditions $\frac{\partial\Phi(Z_{nlj},A_{nlj})}{\partial Z_{nlj}} = 0$ and $\frac{\partial\Phi(Z_{nlj},A_{nlj})}{\partial A_{nlj}} = 0$. Once values Z_{nlj} and A_{nlj} are found to construct the wave function, but we have prefered to use other way, consisting in the addition of a boundary condition. This procedure guarantees a good agreement between all energy levels corresponding to $U(r)$ and $\widetilde{U}(r)$, respectively.
The boundary condition is

$$\int_0^\infty \left[U(r) - \widetilde{U}(r, Z_{nlj}, A_{nlj})\right]\left[\widetilde{F}^2_{nlj}(r) + \widetilde{G}^2_{nlj}(r)\right] dr = 0. \tag{24}$$

If this boundary condition is assumed, then A_{nlj} may be expressed through Z_{nlj} as

$$A_{nlj} = 2\widetilde{\varepsilon}_{nlj} + \int_0^\infty U(r)\left[\widetilde{F}_{nlj}(r) + \widetilde{G}_{nlj}(r)\right] dr.$$

Here the fact that the potential energy $-\frac{Z_{nlj}}{r}$ is two times the total energy $\widetilde{\varepsilon}_{nlj}$ is used.
Substituting A_{nlj} into the expression (23), it is observed that $\Phi(Z_{nlj}, A_{nlj})$ will depend only on Z_{nlj}

$$\Phi(Z_{nlj}) = \int_0^\infty \left[rU(r) + Z_{nlj} - 2r\widetilde{\varepsilon}_{nlj} - rI\right]^2\left[\widetilde{F}^2_{nlj}(r) + \widetilde{G}^2_{nlj}(r)\right] dr, \tag{25}$$

where

$$I \equiv I(Z_{nlj}) = \int_0^\infty U(r)\left[\widetilde{F}_{nlj}(r) + \widetilde{G}_{nlj}(r)\right] dr.$$

To determine the value Z_{nlj} for which $\Phi(Z_{nlj})$, given by (25), has a minimum we use a iterative minimization method [5]. This method quickly converges, with the prescribed accuracy (in few iterative steps), if we start the iteration near an unknown Z_{nlj}. In such a way we can choose as initial value of iteration the effective charge for nonrelativistic case Z_{nl}, [12], as well as the Thomas-Fermi potential [8], for $U(r)$, i.e., the functional (25) has a minimum in the neighborhood of Z_{nl}. The reason for such a choice is that the properties of matter for the considered range of temperatures and densities is approximately described by nonrelativistic quantum physics. We want to remark here that, in order to do this procedure self-consistent, it is necessary to use, in the next iterations, the hydrogenic-like potential (instead of the Thomas-Fermi one).
For the minimization procedure it is assumed that we are able to find the initial value Z_{nl}. Let consider that the fine structure constant $\alpha = \frac{e^2}{\hbar c}$ is approximately equal to zero (extreme non relativistic limit). Then we have the nonrelativistic case [2], [12]

$$-\frac{1}{2}\widetilde{R}''(r) + \left[\widetilde{U}(r) + \frac{l(l+1)}{2r^2}\right]\widetilde{R} = \widetilde{\varepsilon}\widetilde{R}, \text{ where } \widetilde{U}(r) = -\frac{Z_{nl}}{r} + A_{nl}. \tag{26}$$

The functional analogue to (25) is, in this situation

$$\widetilde{\Phi}(Z_{nl}, A_{nl}) = \int_0^\infty \left[rU(r) - r\widetilde{U}(r, Z_{nl}, A_{nl})\right]^2 \widetilde{R}^2_{nl}(r, Z_{nl})\, dr. \tag{27}$$

Moreover, the boundary condition have the form

$$\int_0^\infty \left[U(r) - \widetilde{U}(r)\right]\widetilde{R}^2_{nl}(r)\, dr = 0. \tag{28}$$

The energy levels and radial components for Schrödinger equation are well known [3], [12]. In fact we get

$$\widetilde{\varepsilon}_{nl} = -\frac{Z^2_{nl}}{2n^2} + A_{nl}, \quad \text{and} \quad \widetilde{R}_{nl}(r) = \frac{\sqrt{Z_{nl}}}{n}\sqrt{\frac{(n-l-1)!}{(n+l)!}}x^{l+1}e^{-\frac{x}{2}}L^{2l+1}_{n-l-1}(x), \text{ where } x = \frac{2Z_{nl}r}{n}. \tag{29}$$

Hence (27) becomes the following functional [2], [12]

$$\widetilde{\Phi}(Z_{nl}, A_{nl}) = \frac{1}{2n}\int_0^\infty e^{-x}\left[\frac{nx}{2Z_{nl}}U\left(\frac{nx}{2Z_{nl}}\right) - Z_{nl} + A_{nl}\frac{nx}{2Z_{nl}}\right]^2 xL_{nl}\,dx, \tag{30}$$

where $L_{nl}(x) = \frac{x^{2l+1}}{(n+l)!}(n-l-1)![L_{n-l-1}^{2l+1}(x)]^2$. Using (28) the functional will depend only on Z_{nl}, then the minimum condition ($\frac{d\,\widetilde{\Phi}(Z_{nl})}{d\,Z_{nl}} = 0$) leads us to the equation

$$aZ_{nl}^2 - b(Z_{nl})Z_{nl} + c(Z_{nl}) = 0;$$

where

$$a = \frac{n^2 - l(l+1)+1}{n}, \quad b(Z_{nl}) = \frac{2n^2 - 2l(l+1)+1}{n}(\alpha_0+\beta_0) + (\alpha_1+\beta_1) - \frac{1}{2n}(\alpha_2+\beta_2),$$

$$c(Z_{nl}) = \gamma + \frac{1}{n}[5n^2+1-3l(l+1)]\alpha_0\beta_0 - \frac{1}{2n}(\alpha_0\beta_2+\alpha_2\beta_0), \quad \alpha_k = \int_0^\infty e^{-x}x^kL_{nl}(x)[rU(r)]\,dx$$

with $k = 0,\ 1,\ 2$, and $r = \frac{nx}{2Z_{nl}}$,

$$\beta_k = \int_0^\infty e^{-x}x^kL_{nl}(x)\left[-r\,\frac{d}{dr}(rU(r))\right]dx, \quad \gamma = \int_0^\infty e^{-x}x^kL_{nl}(x)\left[-r\,\frac{d}{dr}(rU(r))rU(r)\right]dx.$$

Taking into account that

$$\int_0^\infty e^{-x}x^kL_{nl}(x)\,dx = 2^kZ_{nl}^{k-1}n^{2-k}\int_0^\infty r^{k-1}\tilde{R}_{nl}^2(r)\,dr,$$

the following equalities

$$\int_0^\infty e^{-x}\frac{1}{x}L_{nl}(x)\,dx = \frac{1}{2l+1}, \quad \int_0^\infty e^{-x}L_{nl}(x)\,dx = 1, \quad \int_0^\infty e^{-x}xL_{nl}(x)\,dx = 2n,$$

$$\int_0^\infty e^{-x}x^2L_{nl}(x)\,dx = 2\left[3n^2 - l(l+1)\right], \int_0^\infty e^{-x}x^3L_{nl}(x)\,dx = 4n\left[5n^2+1-3l(l+1)\right].$$

hold.

Thus our strategy is quite simple: To find Z_{nl} using the iterative method for the following second order equation

$$aZ_{nl}^{(s+1)^2} - b(Z_{nl}^{(s)})Z_{nl}^{(s+1)} + c(Z_{nl}^{(s)}) = 0,$$

in the form

$$Z_{nl}^{(s+1)} = \frac{1}{2a}\left[b(Z_{nl}^{(s)}) + \sqrt{b^2(Z_{nl}^{(s)}) - 4ac(Z_{nl}^{(s)})}\right],$$

putting

$$Z_{10}^{(0)} = Z, \quad Z_{n0}^{(0)} = Z_{n-1\ n-2}, \quad Z_{nl}^{(0)} = Z_{n\ l-1} \quad (l \neq 0).$$

In Figure 1 we provide the scheme of the used algorithm.

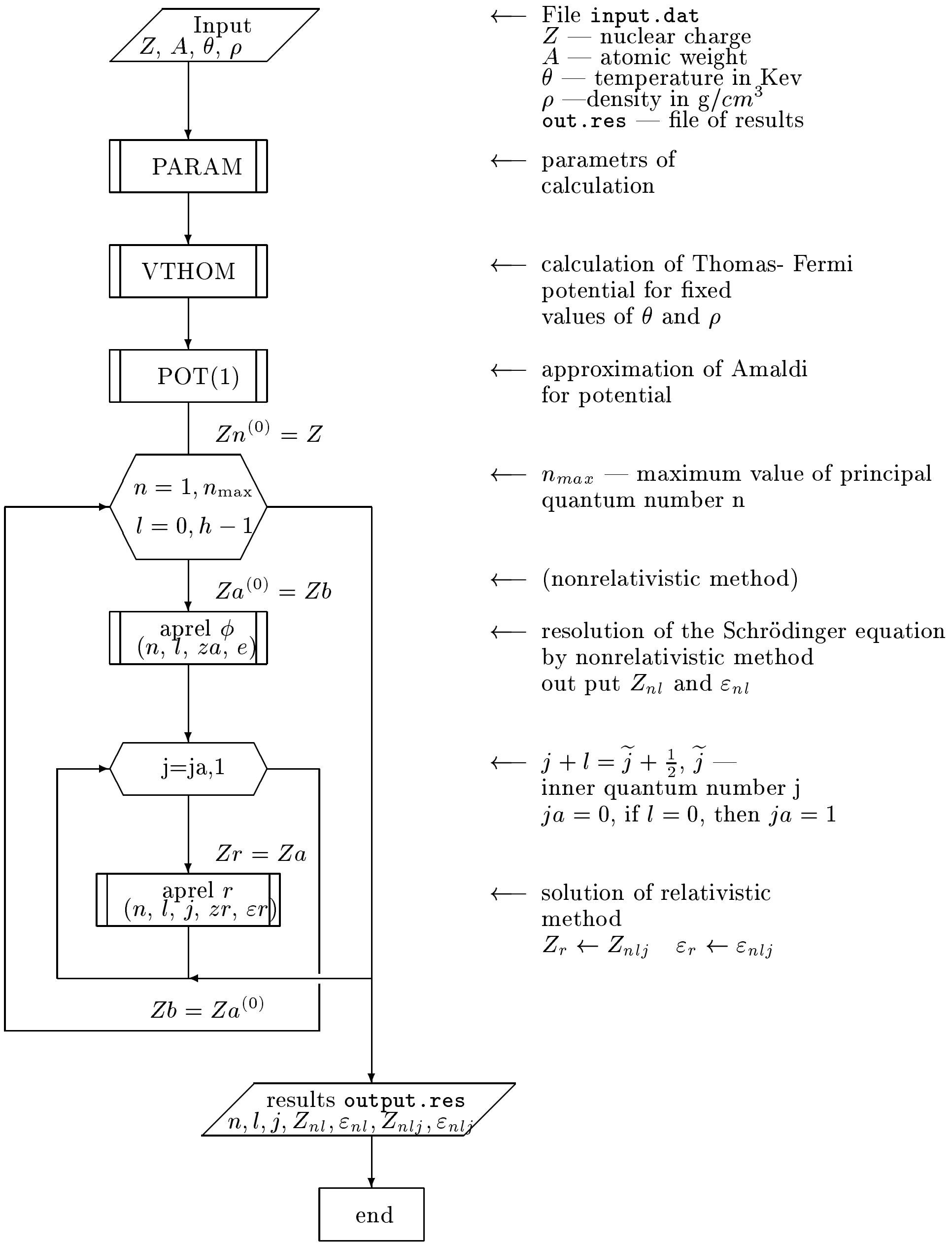

Figure 1: Algorithm for computation of effective charge by relativistic method.

4 Summary of numerical results and conclusions.

To check the quantum-statistical model describing the state of matter in the region of high temperatures, two elements, one of low-Z (aluminium) and other of high-Z (gold), of interest in several physical applications have been employed. The range on temperature and density, for which the model is applicable, covers the region $10^{-3}g/cm^3 \leq \rho \leq 10^2 g/cm^3$, $5ev \leq \theta \leq 15Kev$, depending on the substance and quantum number combinations. However, in this work fixed representative temperatures and densities has been selected. Results from the model are compared with other numerical results.

nlj	$Z_{nl}P$	$Z_{nl}S$	$Z_{nlj}D$	$Z_{nlj}J$	$r_{\max}S$	$r_{\max}D$	$\varepsilon_{nl}P$	$\varepsilon_{nl}S$	$\varepsilon_{nlj}D$	$\varepsilon_{nlj}J$
$10\frac{1}{2}$	12.21	12.50	12.50	12.21	$8.02 \cdot 10^{-2}$	$7.99 \cdot 10^{-2}$	$6.37 \cdot 10^{1}$	$6.37 \cdot 10^{1}$	$6.39 \cdot 10^{1}$	$6.38 \cdot 10^{1}$
$20\frac{1}{2}$	11.18	11.39	11.40	11.18	$4.60 \cdot 10^{-1}$	$4.59 \cdot 10^{-1}$	$1.14 \cdot 10^{1}$	$1.14 \cdot 10^{1}$	$1.14 \cdot 10^{1}$	$1.14 \cdot 10^{1}$
$21\frac{3}{2}$	10.44	10.70	10.70	10.44	$3.74 \cdot 10^{-1}$	$3.74 \cdot 10^{-1}$	$1.04 \cdot 10^{1}$	$1.04 \cdot 10^{1}$	$1.04 \cdot 10^{1}$	$1.04 \cdot 10^{1}$
$32\frac{3}{2}$	9.70	9.81	9.81	9.70	$9.17 \cdot 10^{-1}$	$9.17 \cdot 10^{-1}$	$3.05 \cdot 10^{0}$	$3.05 \cdot 10^{0}$	$3.05 \cdot 10^{0}$	$3.05 \cdot 10^{0}$
$32\frac{5}{2}$	9.70	9.81	9.81	9.70	$9.17 \cdot 10^{-1}$	$9.17 \cdot 10^{-1}$	$3.05 \cdot 10^{0}$	$3.05 \cdot 10^{0}$	$3.05 \cdot 10^{0}$	$3.05 \cdot 10^{0}$
$40\frac{1}{2}$	10.09	10.12	10.12	10.09	$2.43 \cdot 10^{0}$	$2.43 \cdot 10^{0}$	$1.10 \cdot 10^{0}$	$1.09 \cdot 10^{0}$	$1.09 \cdot 10^{0}$	$1.10 \cdot 10^{0}$
$42\frac{5}{2}$	9.37	9.42	9.42	9.37	$2.25 \cdot 10^{0}$	$2.25 \cdot 10^{0}$	$8.82 \cdot 10^{-1}$	$8.84 \cdot 10^{-1}$	$8.84 \cdot 10^{-1}$	$8.82 \cdot 10^{-1}$
$43\frac{5}{2}$	9.12	9.30	9.30	9.12	$1.72 \cdot 10^{0}$	$1.72 \cdot 10^{0}$	$8.12 \cdot 10^{-1}$	$8.12 \cdot 10^{-1}$	$8.13 \cdot 10^{-1}$	$8.11 \cdot 10^{-1}$
$43\frac{7}{2}$	9.12	9.30	9.30	9.12	$1.72 \cdot 10^{0}$	$1.72 \cdot 10^{0}$	$8.12 \cdot 10^{-1}$	$8.12 \cdot 10^{-1}$	$8.13 \cdot 10^{-1}$	$8.11 \cdot 10^{-1}$

Table 1: $Z = 13$. θ=$1.0000 \cdot 10^{-1}$ kev and $\rho = 2.7000 \cdot 10^{-1}$ g/cm^3 given Thomas-Fermi potential, as initial approximation. The energy values and r_{max} are given in atomic units.

nlj	$Z_{nl}P$	$Z_{nl}S$	$Z_{nlj}D$	$Z_{nlj}J$	$r_{\max}S$	$r_{\max}D$	$\varepsilon_{nl}P$	$\varepsilon_{nl}S$	$\varepsilon_{nlj}D$	$\varepsilon_{nlj}J$
$10\frac{1}{2}$	77.89	78.36	78.48	78.12	$1.28 \cdot 10^{-2}$	$1.05 \cdot 10^{-2}$	$2.77 \cdot 10^{3}$	$2.77 \cdot 10^{3}$	$3.08 \cdot 10^{3}$	$3.08 \cdot 10^{3}$
$20\frac{1}{2}$	74.49	75.49	76.42	75.64	$6.94 \cdot 10^{-2}$	$6.02 \cdot 10^{-2}$	$5.53 \cdot 10^{2}$	$5.53 \cdot 10^{2}$	$6.37 \cdot 10^{2}$	$6.37 \cdot 10^{2}$
$21\frac{1}{2}$	72.82	74.38	75.67	74.27	$5.38 \cdot 10^{-2}$	$4.48 \cdot 10^{-2}$	$5.35 \cdot 10^{2}$	$5.36 \cdot 10^{2}$	$6.18 \cdot 10^{2}$	$6.17 \cdot 10^{2}$
$43\frac{7}{2}$	58.39	59.25	59.31	58.43	$2.70 \cdot 10^{-1}$	$2.68 \cdot 10^{-1}$	$8.53 \cdot 10^{1}$	$8.54 \cdot 10^{1}$	$8.57 \cdot 10^{1}$	$8.57 \cdot 10^{1}$
$50\frac{1}{2}$	63.64	63.65	65.13	65.15	$6.27 \cdot \cdot 10^{-1}$	$5.86 \cdot 10^{-1}$	$5.57 \cdot 10^{1}$	$5.55 \cdot 10^{1}$	$6.00 \cdot 10^{1}$	$6.03 \cdot 10^{1}$
$51\frac{1}{2}$	62.12	62.28	63.82	63.42	$6.25 \cdot 10^{-1}$	$5.83 \cdot 10^{-1}$	$5.39 \cdot 10^{1}$	$5.39 \cdot 10^{1}$	$5.82 \cdot 10^{1}$	$5.80 \cdot 10^{1}$
$64\frac{9}{2}$	55.81	55.84	55.86	55.82	$8.37 \cdot 10^{-1}$	$8.35 \cdot 10^{-1}$	$2.87 \cdot 10^{1}$	$2.87 \cdot 10^{1}$	$2.88 \cdot 10^{1}$	$2.88 \cdot 10^{1}$
$65\frac{9}{2}$	55.24	55.43	55.44	55.25	$6.50 \cdot 10^{-1}$	$6.47 \cdot 10^{-1}$	$2.84 \cdot 10^{1}$	$2.84 \cdot 10^{1}$	$2.85 \cdot 10^{1}$	$2.85 \cdot 10^{1}$
$65\frac{11}{2}$	55.24	55.43	55.43	55.25	$6.50 \cdot 10^{-1}$	$6.48 \cdot 10^{-1}$	$2.84 \cdot 10^{1}$	$2.84 \cdot 10^{1}$	$2.84 \cdot 10^{1}$	$2.84 \cdot 10^{1}$

Table 2: $Z = 79$. θ=$1000 \cdot 10^{-1}$ kev and $\rho = 1.9300$ g/cm^3 given Thomas-Fermi potential, as first approximation. The energy values and r_{max} are given in atomic units.

In the next tables are shown the following result corresponding to the gold (Au) and aluminium (Al) for fixed ρ and θ and for some combination of quantum numbers nlj, although we computated for each combination of quantum numbers:

$Z_{nlj}J$ and $\varepsilon_{nlj}J$ — effective charge and energy levels found from our model.
$Z_{nl}S$ and $\varepsilon_{nl}S$ — effective charge and energy levels corresponding to the numerical solutions for Schrödinger equation.
$Z_{nlj}D$ and $\varepsilon_{nlj}D$ — effective charge and energy levels corresponding to the numerical solutions for Dirac equation.
$Z_{nl}P$ and $\varepsilon_{nl}P$ — effective charge and energy levels corresponding to the nonrelativistic cases.
$r_{max}S$ — position of absolute maximum of wave function corresponding to the numerical solution of Schrödinger equation.
$r_{max}D$ — position of absolute maximum of wave function corresponding to the numerical solution of Dirac equation.

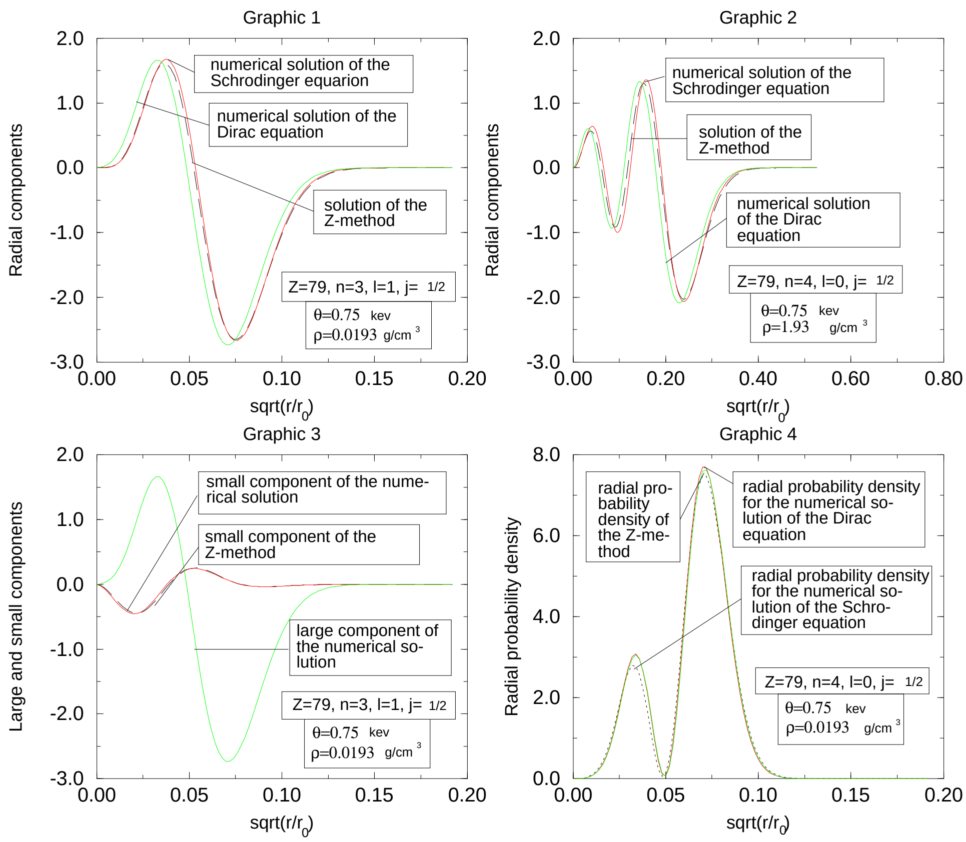

Figure 2: Comparison of numerical results. Here r_0 is the mean value of atomic radius ($r_0 = 1.388(\frac{A}{\rho})^{\frac{1}{3}}$).

Notice the small difference of results compared with several methods. In general, the tendency for high principal quantum number n is the convergence between all methods.

A good agreement between all radial wave functions calculating by several methods for gold are illustrated in the next figures. The large componets are quite similar in all cases. Here our method has called Z-method. It is important to remark that the graphic 3 gives results comparing calculated the small components for Z-method with other one and large radial component of the numerical solution of the Dirac equation. Therefore, we can neglect the influence of the small components to generate opacity calculation code.

In summary, we demostrated that simple formulas for atomic wave functions and energy levels can be used to determine other properties of the matter in very short computational time for any substance at several densities and temperatures. The numerical results show small deviations from numerical solutions for high-Z elements, which is balanced by the simplicity and rapidity of the computations, and for low atoms is regarded complete coincidence of the wave functions, calculated with help of different methods. In this way the model can be used in the opacity and equation of state calculations scheme, because it has a wide flexibility depending on plasma conditions.

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