

One-electron processes in atomic physics

Author: Víctor Camí Núñez.

Facultat de Física, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain.

Advisor: Francesc Salvat Gavaldà

Abstract: In this work we have developed a Fortran 77 subroutine package to solve numerically the radial Schrödinger equation. We have also defined an adjustable radial grid with specific characteristics that permit solving the radial Schrödinger equation. The numerical method implemented is the Hamming predictor-corrector method that is started by expanding the solution at the first four point as a power series. Furthermore, using that package, we have computed the mean-life for spontaneous emissions between bound energy levels using a Coulomb potential with and without screening.

I. INTRODUCTION

The solution of the radial Schrödinger equation during the Physics degree was restricted to the use of Coulomb potential and hydrogenic models because in this case the radial Schrödinger equation can be solved analytically and its expressions are tabulated. However, for potentials different from the Coulomb potential, the solution of the radial Schrödinger equation cannot be found analytically. Then it is necessary to solve the radial Schrödinger equation numerically. In this work, we have developed a Fortran subroutine package named SCHBND, which implements the Hamming predictor-corrector method [1], to solve numerically the radial Schrödinger equation. We have validated its accuracy by comparing the energy eigenvalues calculated with SCHBND with the ones generated by the subroutine package RADIAL [2] which also solves the radial Schrödinger equation to high accuracy and it has been provided for my advisor. As an application of SCHBND, first, we expose a brief description of stimulated absorption, stimulated emission and spontaneous emission for bound states. For spontaneous emission, we have written a program which computes the mean-lives for different screened Coulomb potentials and energy levels. We consider the case of gross structure, that is, non-relativistic electron for spin-less particles.

All the atoms, except hydrogen, are multi-electronic atoms. Even though, we use the independent-particle model which means that the interactions among the different electrons is non-existent or negligible, we just consider the one-electron transitions. Hence, all the expressions of this work apply to one-electron atoms.

We present the results of mean-lives calculated for different atomic numbers Z for a Coulomb potential and for a Coulomb potential with the Thomas-Fermi-Moliere (TFM) screening function. We also analyze the effect of screening on the mean-lives. To evaluate the effect of screening on the mean-life we consider the screened Coulomb potential

$$V(r) = \frac{-Ze^2}{r}\phi(r), \quad (1)$$

where ϕ is the TFM screening function.

$$\phi(r) = 0.10e^{-6r/b} + 0.55e^{-1.2r/b} + 0.35e^{-0.3r/b} \quad (2a)$$

$$b = 0.88534a_0Z^{-1/3} \quad (2b)$$

For high values of r , the charge of the nucleus is completely screened and the number of bound energy levels is finite. This happens because the potential includes the self-screening of the electron which suffers the transition. We introduce the Latter's tail correction [3] to eliminate this self-screening,

$$rV(r) = \begin{cases} -Ze^2\phi(r) & \text{if } rV(r) < -e, \\ -e & \text{otherwise.} \end{cases} \quad (3)$$

The use of a Coulomb potential with a screening functions conflicts with the use of the independent-particle model. Despite this, we have use screened Coulomb potentials to do a first estimation about how mean-lives are modify by the inclusion of a screening.

II. NUMERICAL SOLUTION OF THE RADIAL SCHRÖDINGER EQUATION

In this section all the expressions are in atomic units. The SCHBND subroutine package solves the radial Schrödinger equation for bound states for a central potential $V(r)$ such that the function $\mathcal{V}(r) = V(r)r$ is finite for all the values of r and it tends to constant values when $r \rightarrow \infty$ and $r \rightarrow 0$. We consider central-field orbitals of the form

$$\psi_{n\ell m}(\mathbf{r}) = \frac{P_{n\ell}(r)}{r} Y_{\ell m}(\mathbf{r}), \quad (4)$$

whose radial part satisfies the second-order differential equation

$$P_{n\ell}''(r) + 2 \left[E_{n\ell} - V(r) - \frac{\ell(\ell+1)}{2r^2} \right] P_{n\ell}(r) = 0, \quad (5)$$

where $P_{n\ell}(r)$ is the reduced radial wave with boundary conditions $P_{n\ell}(0) = 0$ and $P_{n\ell}(\infty) = 0$ and it is normalized to unity. $P_{n\ell}(r)$ has a number of zeros equal the radial quantum number $n_r = n - (\ell + 1)$.

A. Defining the grid of points

In the numerical solution we consider a radial grid, $r_i (i = 1, \dots, N)$, whose a spacing $\Delta_i = r_{i+1} - r_i$ should increase monotonously to have a dense enough grid near the origin where $P(r)$ changes its value swiftly. Moreover, the distance between two consecutive points has to be smaller than the distance between two consecutive zeros of $P(r)$. The grid covers the interval $(r = 0, r_N)$, for $r > r_N$ the contribution of $P(r)$ can be neglected. Other parameters are r_2 which determines the spacing for lower radii and $\Delta_N = r_N - r_{N-1}$ which defines the spacing for high radii. We introduce the transformation $x = g(r)$ to obtain a grid with uniform spacing with $x = 1, \dots, N$.

$$x = g(r) = ar + b \ln(c + r) + d. \quad (6)$$

Then, the grid of radii is obtained by solving Eq.(7) using the bisection method.

$$ar_i + b \ln(c + r_i) + d = i \quad i = 1, 2, \dots, N. \quad (7)$$

The values of the parameters a, b, c and d are obtained by solving the system of equations

$$\begin{aligned} b \ln(c) + d = 1, \quad a r_N + b \ln(c + r_N) + d = N, \\ a + \frac{b}{c} = \frac{1}{r_2}, \quad a + \frac{b}{c + r_N} = \frac{1}{\Delta_N}. \end{aligned} \quad (8)$$

When the value

$$A_{\text{grid}} \equiv \frac{r_N - (N-1)r_2}{r_N} \frac{\Delta_N}{\Delta_N - r_2}. \quad (9)$$

lies in the interval $(0.5, 1)$ the system of equations Eq.(8) has a unique solution given by

$$\begin{aligned} c = x r_N, \quad b = \frac{x(c + r_N)(\Delta_N - r_2)}{\Delta_N r_2}, \\ a = \frac{c - b r_2}{c r_2}, \quad d = 1 - b \ln c, \end{aligned} \quad (10)$$

where x is the positive root of

$$(x+1) \left[1 - x \ln \left(\frac{x+1}{x} \right) \right] = A_{\text{grid}} \quad (11)$$

which is solved again by the bisection method.

B. SCHBND package

SCHBND package solves the radial Schrödinger equation as a system of first order equations in vector form using the Hamming predictor-corrector method.

$$\frac{d\mathbf{Y}}{dr} = \mathbf{F}[r, \mathbf{Y}], \quad (12)$$

$$\mathbf{Y}(r) = \begin{pmatrix} P(r) \\ Q(r) \end{pmatrix}, \quad \frac{d\mathbf{Y}}{dr} = \begin{pmatrix} 0 & 1 \\ 2(U_\ell - E) & 0 \end{pmatrix} \mathbf{Y}(r), \quad (13)$$

where

$$U_\ell(r) = V(r) + \frac{\ell(\ell+1)}{2r^2}. \quad (14)$$

Hamming's method assumes a uniform grid with spacing H . To do that, Eq.(12) is subject to the change variable $x = g(r)$.

$$\frac{d\mathbf{Y}}{dx} = \frac{1}{g'(r)} \mathbf{F}[r, \mathbf{Y}] \equiv \mathbf{F}[x, \mathbf{Y}]. \quad (15)$$

Then, the solution at the next point $x_{i+1} = x_i + H$ is obtained using Hamming predictor-corrector method which consists in five stages:

1) Predictor:

$$\mathbf{P}_{i+1} = \mathbf{Y}_{i-3} + \frac{4H}{3} (2\mathbf{Y}'_i - \mathbf{Y}'_{i-1} + 2\mathbf{Y}'_{i-2}).$$

2) Modificator:

$$\mathbf{M}_{i+1} = \mathbf{P}_{i+1} - \frac{112}{121} (\mathbf{P}_i - \mathbf{C}_i),$$

$$\mathbf{M}'_{i+1} = \mathbf{F}(x_{i+1}, \mathbf{M}_{i+1}).$$

3) Corrector:

$$\mathbf{C}_{i+1} = \frac{1}{8} [9\mathbf{Y}_i - \mathbf{Y}_{i-2} + 3H (\mathbf{M}'_{i+1} + 2\mathbf{Y}'_i - \mathbf{Y}'_{i-1})].$$

4) Final value:

$$\mathbf{Y}_{i+1} = \mathbf{C}_{i+1} + \frac{9}{121} (\mathbf{P}_{i+1} - \mathbf{C}_{i+1}) + O(H^6).$$

Where $\mathbf{Y}_i \equiv \mathbf{Y}(r_i)$ and $\mathbf{Y}'_i \equiv \mathbf{F}[x_i, \mathbf{y}_i]$. In this way we can obtain the values of $P(r)$ and $Q(r) = P'(r)$ in all the points of the grid, the last step is to normalize $P(r)$ and $Q(r)$.

The main advantage of that method is that is stable and the error decreases in the direction in which \mathbf{Y}_i increases in magnitude. However, this is not a self-starting method. To start it are needed the first four point which are obtained following the same procedure implemented in RADIAL package, section II C.

The solution can start from the grid point $r = 0 (r = r_N)$ which is called the outward(inward) solution. In fact, the inward solution starts in the practical infinity, r_∞ , which is the point that fulfills the condition

$$r_\infty \mu(r_\infty) > 60, \quad (16)$$

where $\mu(r)$ is given by WKB approximation [4]

$$\mu(r) \equiv \sqrt{V(r) + \frac{\ell(\ell+1)}{2r^2}}. \quad (17)$$

Inward solution starts in r_∞ instead of r_N because $P(r_N)$ could be quite small if r_N is far enough from the origin. The error introduced changing the start point of the inward solution can be neglected and it is established that $P(r) = 0$ for $r > r_\infty$. In the rest of this work we have considered that $r_N = r_\infty$.

C. RADIAL subroutine package

RADIAL computes the values of $P(r)$ and $Q(r)$ in the interval (r_a, r_b) where r_a and r_b are points of the grid and the values of $P(r_a)$ and $Q(r_a)$ are already known. The values of $\mathcal{V}(r) = V(r)r$ have been interpolated in this interval by a cubic polynomial

$$\mathcal{V}(r) = V(r)r = v_0 + v_1r + v_2r^2 + v_3r^3. \quad (18)$$

To start the inward solution it is necessary to know the value of $P(r_N)$ and $Q(r_N)$, we estimated them using the WKB approximation.

$$P(r_N) = 1 \quad \text{and} \quad \frac{Q(r_N)}{P(r_N)} = -\frac{\mu'(r_N)}{2\mu(r_N)} - \mu(r_N). \quad (19)$$

Introducing the change of variables $x \equiv (r - r_a)/h$ and $h \equiv r_b - r_a$, $P(x)$ is expanded as a power series in x and it is obtained the recurrence relation

$$P(x) = \sum_{k=0}^{\infty} A_k x^k, \quad (20)$$

$$\begin{aligned} A_k = & \frac{h}{k(k-1)r_a} [-2(k-1)(k-2)A_{k-1} \\ & + \frac{h}{r_a} \{(u_0 - (k-2)(k-3))A_{k-2} + u_1A_{k-3} \\ & + u_2A_{k-4} + u_3A_{k-5} + u_4A_{k-6}\}], \end{aligned} \quad (21)$$

where $A_0 = P(r_a)$, $A_1 = hP'(r_a)$, $A_k = 0$ if $k < 0$ and where

$$\begin{aligned} u_0 &= \ell(\ell+1) + 2v_0r_a + 2(v_1 - E)r_a^2 + 2v_2r_a^3 + 2v_3r_a^4, \\ u_1 &= 2[v_0 + 2(v_1 - E)r_a + 3v_2r_a^2 + 4v_3r_a^3]h, \\ u_2 &= 2[(v_1 - E) + 3v_2r_a + 6v_3r_a^2]h^2, \\ u_3 &= 2(v_2 + 4v_3r_a)h^3, \\ u_4 &= 2v_3h^4. \end{aligned} \quad (22)$$

For $x = 1$ the values of $P(r_b)$ and $Q(r_b)$ are,

$$P(r_b) = \sum_{k=0}^{\infty} A_k, \quad Q(r_b) = h^{-1} \sum_{k=0}^{\infty} kA_k. \quad (23)$$

The outward solution starts with the condition $P(r_1) = 0$ and $Q(r_1) = 0$, the outward solution begins with $r_a = 0$, to avoid possible divergences the power expansion is modified

$$P(x) = x^s \sum_{k=0}^{\infty} A_k x^k, \quad (24)$$

$$A_k = \frac{u_1A_{k-1} + u_2A_{k-2} + u_3A_{k-3} + u_4A_{k-4}}{(s+k)(s+k-1) - u_0}, \quad (25)$$

where $s = (\ell + 1)$ and $A_0 = 1$. The last step is to normalize the values of $P(r)$ and $Q(r)$. The program adds as many terms of the summation as needed to ensure that the relative error in the sum is lower than a certain value of tolerance $\epsilon \sim 10^{-13}$.

D. The shooting method

The solution of the radial Schrödinger equation is started by introducing an estimate of the energy eigenvalue E between the values

$$\begin{aligned} E_{\text{inf}} &\simeq \min \left\{ V(r) + \frac{\ell(\ell+1)}{2r^2} \right\}, \\ E_{\text{sup}} &\equiv V(r_N) + \frac{\ell(\ell+1)}{2r_N^2}. \end{aligned} \quad (26)$$

We consider a matching point r_m that is larger than the outer turning point and beyond the classical inflection point of $P(r)$. This means that all zeros of $P(r)$ lie in the interval $(0, r_m)$. This point is determined by the condition

$$V(r_i) > E - \frac{\ell(\ell+1)}{2r_i^2} \quad \text{if} \quad i \geq m. \quad (27)$$

The outward solution starts computing the values of $P(r)$ and $Q(r) = P'(r)$ in the interval $(0, r_m)$ using a value of the energy $E = (E_{\text{inf}} + E_{\text{sup}})/2$. The numbers of zeros of $P(r)$ is equal to the number of times that $P(r)$ changes its sign. If the number of zeros is lower(greater) than n_r E replaces $E_{\text{inf}}(E_{\text{sup}})$. This process is repeated until it is found a value of E with n_r zeros. This strategy is consistent provided that there is at most one zero between two consecutive points of the grid, to ensure that, it is necessary a dense enough grid. Then, the inward solution is computed from r_N to r_m . To connect the inward, P_{in} , and the outward, P_{out} , solutions it is necessary to re-normalize both solutions so that $P_{\text{in}}(r_m) = P_{\text{out}}(r_m)$. Then, $P(r)$ is continuous in the interval (r_1, r_N) . $Q(r)$ should also be continuous in r_m , otherwise the value of the energy is corrected using the Mayer's correction [5]

$$\Delta E = P(r_m)[Q_{\text{out}}(r_m) - Q_{\text{in}}(r_m)] \left[2 \int_0^{\infty} P^2(r) dr \right] \quad (28)$$

Then, the value of the energy eigenvalue is modified, $E_{n\ell} = E + \Delta E$. The process is repeated until $Q(r)$ is continuous in r_m . The last step is to normalize $P(r)$.

E. Analysis of the SCHBND results

To estimate the accuracy of SCHBND, we have computed energy eigenvalues for different energy levels for atoms of Au, Al and Ag using a Coulomb potential with a TFM screening function. We have compared that values with the ones provided by RADIAL. The energy eigenvalues obtained using SCHBND are slightly less accurate than the ones given by RADIAL. The relative difference is smaller when the number of grid points is increased and the relative difference reaches a constant value for a determined number of grid points.

	Al(1s)	Ag(1s)	Au(1s)	Al(3p)	Ag(5s)	Au(5d)
NGP	$\Delta E(\%)$	$\Delta E(\%)$	$\Delta E(\%)$	$\Delta E(\%)$	$\Delta E(\%)$	$\Delta E(\%)$
250	1E-3	2E-3	2E-3	1E-2	2E-1	5E-1
500	2E-6	2E-6	4E-6	1E-3	6E-3	1E-4
1000	1E-7	1E-6	4E-6	1E-3	2E-3	6E-5
5000	1E-7	1E-6	4E-6	8E-6	1E-4	3E-5
10000	1E-7	1E-6	4E-6	1E-7	1E-5	4E-6
20000	1E-7	1E-6	4E-6	1E-7	5E-6	1E-7
25000	1E-7	1E-6	4E-6	1E-7	5E-6	1E-7

TABLE I: Values of the relative difference between the energy eigenvalue provided by RADIAL and by SCHBND package (ΔE) for Al, Ag and Au.

III. APPLICATION: ABSORPTION AND EMISSION OF RADIATION

A. Semiclassical theory

We consider an atom with just one electron which interacts with the electromagnetic radiation in a region free of other charges. This atom can be in the quantum bound state $|\psi_b\rangle$ with energy E_b or in $|\psi_a\rangle$ with energy E_a . The pulse has a wave vector \mathbf{k} , polarization $\hat{\boldsymbol{\epsilon}}$ and density of photons per unit volume and per unit frequency $n(\omega)$ with $\omega = ck$.

First, we consider the case of absorption. In a transition from $|\psi_a\rangle$ to another state $|\psi_b\rangle$ with $E_a < E_b$, the atom absorbs a photon of the pulse with frequency $\omega_{ba} = (E_b - E_a)/\hbar$. The transition rate for absorption [6] is given by

$$W_{ba}(\hat{\mathbf{k}}, \hat{\boldsymbol{\epsilon}}) = n(\omega) \frac{(2\pi ec)^2}{\hbar\omega_{ba}} \left| M_{ba}(\hat{\mathbf{k}}, \hat{\boldsymbol{\epsilon}}) \right|^2 \delta(\omega_{ba} - \omega), \quad (29)$$

where e is the electron charge, c is the speed of light and

$$M_{ba}(\hat{\mathbf{k}}, \hat{\boldsymbol{\epsilon}}) = \langle \psi_b | \frac{1}{m_e c} e^{i(\mathbf{k}\cdot\mathbf{r})} \hat{\boldsymbol{\epsilon}} [\mathbf{p} + i\frac{\hbar}{2} \boldsymbol{\sigma} \times \mathbf{k}] | \psi_a \rangle, \quad (30)$$

where m_e is the mass of the electron, $\boldsymbol{\sigma}$ are the Pauli matrices. Assuming that the radiation is incoherent, the transition rate has to be integrated over all the frequencies. Considering the case in which the wavelength $\lambda = 2\pi/k$, is much longer than the atomic radius, the exponential in Eq.(30) can be approximated by unity. Moreover, we can neglect the effect of the spin term to arrive at the dipole approximation:

$$M_{ba} = \frac{1}{m_e c} \hat{\boldsymbol{\epsilon}} \langle \psi_b | \mathbf{p} | \psi_a \rangle = ik\hat{\boldsymbol{\epsilon}} \langle \psi_b | \mathbf{r} | \psi_a \rangle, \quad (31)$$

For isotropic and non-polarized radiation, the absorption rate is

$$W_{ba} = n(\omega_{ba}) \frac{4\pi^2 e^2}{3\hbar} \omega_{ba} |\langle \psi_b | \mathbf{r} | \psi_a \rangle|^2. \quad (32)$$

This expression also give the transition rate for stimulated emission from $|\psi_a\rangle$ to a lower state $|\psi_b\rangle$ with $E_a > E_b$ in which the atom emits a photon with ω_{ba} .

The transition rate for spontaneous emission from $|\psi_a\rangle$ ($a = n\ell$) to $|\psi_b\rangle$ ($b = n'\ell'$) with quantum numbers $n\ell$ and $n'\ell'$ respectively is [6]

$$W_{ba}^s = \frac{\omega_{ba}^2}{\pi^2 c^3} \frac{W_{ba}}{n(\omega_{ba})} = \frac{4e^2}{3\hbar c^3} \omega_{ba}^3 |\langle \psi_b | \mathbf{r} | \psi_a \rangle|^2. \quad (33)$$

Instead of transitions between individual states, what is observed are the transition between bound the energy levels E_a and E_b . Within the dipole approximation it is customary to introduce the oscillator strength, a dimensionless quantity defined as

$$f_{ba} \equiv \frac{2m_e}{3\hbar} \omega_{ba} |\langle \psi_b | \mathbf{r} | \psi_a \rangle|^2. \quad (34)$$

The average oscillator strength is defined as

$$\overline{f_{ba}} \equiv \frac{1}{2\ell + 1} \sum_{m_L = -\ell}^{\ell} \sum_{m'_L = -\ell'}^{\ell'} f_{ba} \quad (35)$$

That is, as a sum of oscillator strengths over the degenerated states in the final level and an average over states of the initial level.

From Eq.(34) and Eq.(35),

$$\overline{f_{ba}} = \frac{2m_e}{3\hbar} \omega_{ba} \left| \int_0^{+\infty} P_{n'\ell' r} P_{n\ell} dr \right|^2 \langle 1\ell 0 | \ell' 0 \rangle^2, \quad (36)$$

where $\langle 1\ell 0 | \ell' 0 \rangle$ is the Clebsch-Gordan coefficient. Thus, the transition rate for spontaneous emission is expressed as

$$\overline{W_{ba}^s} = \frac{2e^2}{m_e c^3} \omega_{ba}^2 \overline{f_{ba}}. \quad (37)$$

If we consider that we have an initial number of atoms, $N(0)$, in the excited level E_a . The number of atoms that remain excited after a time t is

$$N(t) = N(0) \exp\left(-\frac{t}{\tau}\right). \quad (38)$$

The mean-life is the rate of decrease of the population of that level to all the possible levels which lower energy permitted by the selection rules.

$$\tau = \left(\sum_b W_{ba}^s \right)^{-1} = (\overline{W_{ba}^s})^{-1}. \quad (39)$$

IV. VALUES OF MEAN-LIVES COMPUTED

A. Coulomb potential

We have calculated the mean-lives of hydrogen for different energy levels and we have seen that these values are in good agreement with those in Ref.[7].

nl	2s	2p	3s	3p	3d	4s	4p
$(\tau/s) \times 10^8$	∞	0.1596	15.839	0.5271	1.5467	22.657	1.2305

TABLE II: Mean-lives of energy levels for hydrogen for a Coulomb potential.

Moreover, we have verified that the hydrogenic scaling property

$$\tau(Z) = \frac{\tau(Z=1)}{Z^4}, \quad (40)$$

is satisfied.

	$(\tau/s) \times 10^8$					
	2p	3s	3p	3d	4s	4p
He	9.98E-3	9.90E-1	3.29E-2	9.67E-2	1.42E+0	7.69E-2
C	1.23E-4	1.22E-2	4.07E-4	1.19E-3	1.75E-2	9.49E-4
Ne	1.60E-5	1.58E-3	5.27E-5	1.55E-4	2.27E-3	1.23E-4
Al	5.59E-6	5.55E-4	1.85E-5	5.42E-5	7.93E-4	4.31E-5
Ar	1.52E-6	1.51E-4	5.02E-6	1.47E-5	2.16E-4	1.17E-5
Kr	9.50E-8	9.43E-6	3.14E-7	9.21E-7	1.35E-5	7.33E-7

TABLE III: Half-lives for different atoms and energy levels for a Coulomb potential. The mean-life of energy level 2s is infinite.

B. Screening Coulomb potential

We have introduced the TFM screening function to the Coulomb potential and we have computed the mean-lives for the same atoms and energy levels of Table III. The screening reduces the energy $|E|$ of the level. As a consequence, there is a reduction of the frequency of the emitted photon. Moreover, the oscillator strength also suffers a variation because it depends on the frequency of the photon. As a result, the transition rate is smaller, this produces an increase of the mean-life of that level.

	$(\tau/s) \times 10^8$					
	2p	3s	3p	3d	4s	4p
He	1.32E-1	7.21E+0	4.23E-1	1.55E+0	1.12E+1	9.78E-1
C	1.00E-2	4.21E+0	2.94E-2	1.38E+0	1.08E+1	6.85E-2
Ne	8.62E-5	1.79E-1	3.39E-3	2.36E+0	5.95E-1	1.03E-2
Al	1.85E-5	2.50E-2	2.11E-3	2.71E+0	1.13E-1	6.35E-3
Ar	3.54E-6	1.54E-3	9.74E-5	1.01E+0	2.51E-2	7.27E-4
Kr	1.46E-7	2.88E-5	9.76E-7	5.54E-6	1.69E-4	1.21E-5

TABLE IV: Mean-lives for different atoms and energy levels using a Coulomb potential with a TFM screening function. The mean-life of energy level 2s is infinite.

V. CONCLUSIONS

We have implemented the Hamming predictor-corrector method to solve the radial Schrödinger equation numerically. We have also seen how important is choosing the radial grid to evaluate correctly the values of $P(r)$ and the energy eigenvalue, and to not skip any zero of the function. Moreover, we have verified the values of $P(r)$ and $E_{n\ell}$ developing a program which computes the mean-lives for hydrogenic atoms and seeing that the values are compatible with the ones in [7] and verify Eq.(40). Then, we have introduced the TFM screening function to the Coulomb potential and we have seen that screening produces a reduction of the transition rate and, as a consequence, the mean-life of the level increases.

Acknowledgments

I would like to thank Francesc Salvat Gavaldà for his time and dedication during the realization of this work and to my family for their support.

[1] R.W. Hamming "Stable Predictor-Corrector Methods for Ordinary Differential Equations" Journal of the ACM (JACM), **6** (1959) 37 - 47
[2] F. Salvat and J. M. Fernandez-Varea. "RADIAL: a Fortran subroutine package for the solution of the radial Schrodinger and Dirac wave equations". Internal report, University of Barcelona, 2015.
[3] Latter, R. (1955) "Atomic energy levels for the Thomas-Fermi and Thomas-Fermi-Dirac potential." Phys. Rev. **99**, 510-519.

[4] Sakurai J.J. "Modern quantum mechanics" (AW, 1994)
[5] Mayers, D.F. (1957), "Relativistic self-consistent field calculations for mercury." Proc. Roy. Soc. (London) A241, 93-98.
[6] Francesc Salvat, "Física atòmica i radiació". Barcelona. Otoño 2015
[7] Bethe H.A., Salpeter E.E. "Quantum mechanics of one- and two-electron atoms" (Springer, 1957)