Construction of an Advanced Algorithm to Solve Fundamental Differential equations

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Overview

Collaborators: OPRA-project Research Team

- Theocharis Kosmas, Univ. of Ioannina, Greece: S.C. of the Project OPRA-UoI-UoJ
- Jouni Suhonen, Univ. of Jyvaskyla, Finland: Leader of testing QED and BSM theories
- Odyssefs Kosmas (Principal Investigator), ConIgital, Manchester, Coventry, UK: Leading the derivation and assessment of the new algorithms
- Dimitrios Papoulias (PostDoc), Univ. of Athens, Greece: Testing QED and BSM theories with the new algorithms
- Athanasios Gkrepis (PhD St), derivation and assessment of the new algorithms (in Python language)
- Theodora Papavasileiou (PhD St), testing QED theory with the new algorithms
- Leandros Perivolaropoulos (Deputy Scientific Coordinator), Univ. of Ioannina, Greece

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OPRA

The basic tools for the quantum mechanical description in the microcosm are the wavefunctions. They contain all the information of the underlying quantum system. They are solutions of differential equations ordinary (ODEs) or partial (PDEs) (Schrödinger, Klein Gordon, Dirac, Breit-Darwin...).

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Such equations in their majority cannot be solved analytically. So the development of advanced (numerical) methods for solving them is a necessity.

These methods can generally be categorized as

- deterministic
- stochastic

The 3-D time-independent Schrödinger equation, (for a symmetric potential $V(|x|)$) is

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In spherical coordinates (r, θ, ϕ), this equation is equivalently written as,

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi + V(r)\psi = E\psi.$$

Separation of spherical coordinates

As is well known, assuming that:

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As is well known, assuming that:

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(i.e. using separation of radial from the angular part) we obtain,

$$\left[\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r) - \frac{2\mu r^2}{\hbar^2}\left[V(r)-E\right]\right] + \left[\frac{1}{Y(\theta,\phi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi) + \frac{1}{Y(\theta,\phi)\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi)\right] = 0.$$

In the latter equation we have the sum of two terms, with the first term depending explicitly on variable r and the second term on the angular variables.

This can only happen if both of these terms are constants.For quantum mechanical reasons, we choose these constants to be proportional to $l(l+1)$, where $l = 0, \ldots, n-1$, i.e.

Radial equation

$$\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r) - \frac{2\mu r^2}{\hbar^2}\left[V(r) - E\right] = l(l+1)$$

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and

Angular equation

$$\frac{1}{Y(\theta,\phi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi) + \frac{1}{Y(\theta,\phi)\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi) = -l(l+1)$$

which are called the radial and angular equations respectively.

Using again the method of separation of variables on the angular equation $Y(\theta,\phi) = f(\theta)g(\phi)$,

$$\frac{1}{Y(\theta,\phi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi) + \frac{1}{Y(\theta,\phi)\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi) = -l(l+1)$$

we obtain the following equation

$$\frac{\sin\theta}{f(\theta)}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta) + l(l+1)\sin^2\theta + \frac{1}{g(\phi)}\frac{\partial^2}{\partial\phi^2}g(\phi) = 0.$$

Again now, using the same logical reasoning as before we obtain the following equations.

$$\frac{\sin\theta}{f(\theta)}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta)+l(l+1)\sin^2\theta=m^2$$

and

$$\frac{1}{g(\phi)}\frac{\partial^2}{\partial\phi^2}g(\phi)=-m^2.$$

The second equation is a linear second order differential equations which admits solutions of the form,

$$g(\phi)=e^{im\phi}.$$

As for the first equation, it admits solutions of the form

$$f(\theta) = P_{l,m}(\cos\theta)$$

where $P_{l,m}$ are the associated Legendre polynomials which can be generated using the following formula,

$$P_{l,m}(x) = (-1)^m \sqrt{(1-x^2)^m} \frac{d^m}{dx^m} P_l(x) \quad \text{where} \quad P_l(x) = \frac{(-1)^l}{2^l l!} \frac{d^l}{dx^l} (1-x^2)^l.$$

So the solutions of the angular equation are,

$$Y_{l,m}(\theta, \phi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_{l,m}(cos\theta)e^{im\phi}$$

which are called spherical harmonics. The coefficient in front is comes from the orthonormalization condition, i.e.,

$$\int_0^{\pi} \int_0^{2\pi} Y^*_{l,m} Y_{l',m'} = \delta_{l,l'}\delta_{m,m'},$$

where δ denotes the Kronecker delta symbol ($\delta_{i,j} = 1$ if $i = j$, else 0).

The radial equation,

$$\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r)-\frac{2mr^2}{\hbar^2}\left[V(r)-E\right]=l(l+1)$$

using the transformation $R(r)=u(r)/r$, provides the known as "reduced radial equation",

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}u(r)+V(r)u(r)-Eu(r)-\frac{l(l+1)}{r^2}u=0.$$

Assuming that, V has the simple Coulomb potential form,

$$V(r) = -\frac{e^2}{r}$$

the normalized analytic solution of the radial part of the wavefunction is given by,

$$R_{n,l}(r) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}} e^{-r/na_0} \left(\frac{2r}{na_0}\right)^l \mathcal{L}_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)$$

where $\mathcal{L}_j^i$ are the associated Laguerre polynomials $\mathcal{L}_j^i$, which satisfy the following equation,

$$x\mathcal{L}_j^{i''}(x) + (1-x-i)\mathcal{L}_j^{i'}(x) + j\mathcal{L}_j^i(x) = 0.$$

Beginning with the two-body purely leptonic system (e.g. muonium, positronium), we can calculate its Bohr radius a_0 using the formula,

$$a_0 = \frac{\hbar}{\mu a}$$

where μ is the reduced mass of the two body system. The energy eigenvalue is given by the formula

$$E_n = -\frac{\hbar^2}{2\mu a_0^2 n^2}.$$

Solution of the Schrödinger Differential equation using NNT

Going back to the reduced radial equation,

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}u(r) + V(r)u - Eu(r) = 0,$$

if u is a solution of the latter ODE, by considering a grid $r_1, r_2, \ldots, r_s$, it also holds,

$$\sum_{i=1}^{s}\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}u(r_i) + V(r_i)u(r_i) - Eu(r_i)\right]^2 = 0$$

Then we define as

$$F_{err}(u) = \sum_{i=1}^{s}\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}u(r_i) + V(r_i)u(r_i) - Eu(r_i)\right]^2$$

the so called error function.

Defining,

$$u = re^{-kr}N(r, u, v, w)$$

where f is the logistics function,

Logistics function

$$f(x) = \frac{1}{1 + e^{-x}}$$

and N is the function, given by

$$N(r, u, v, w) = \sum_{i=1}^{m} v_i f(w_i r + u_i)$$

we have created a 2-layers N.N. with activation function the logistics function.

Creation of the Neural Network

- Our approach to solve the reduced radial equation consists in parametrizing u(r) and then minimizing the left-hand side of equation,

$$\sum_{i=1}^{s}\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}u(r_i)+V(r_i)u(r_i)-Eu(r_i)\right]^2=0$$

- As to avoid the trivial solution u(r) $= 0$ everywhere, we can divide by the normalization $\int u^2(r)dr$.
- We use the parametrization

$$u(r)=re^{-kr}N(r,u,w,v),k>0,$$

where N(r, u, w, v) is a feed-forward artificial neural network with

- two hidden layers
- one input unit (r)

The Neural Network Technique

- The biases are denoted by $u = (u_1, u_2, \ldots, u_m)$, where m denotes the number of hidden units.
- The weights to the hidden layers are denoted by $w = (w_1, w_2, ..., w_m)$ and
- the weights to the output by $v = (v_1, v_2, ..., v_m)$.
- The hidden layer units have sigmoid activations of the form $f(x) = (1 + e^{-x})^{-1}$.

Finally we have

$$N(r, u, w, v) = \sum_{i=1}^{m} v_i f(w_i r + u_i)$$

To obtain the precise expression for the reduced radial wavefunction u(r) we follow the steps:

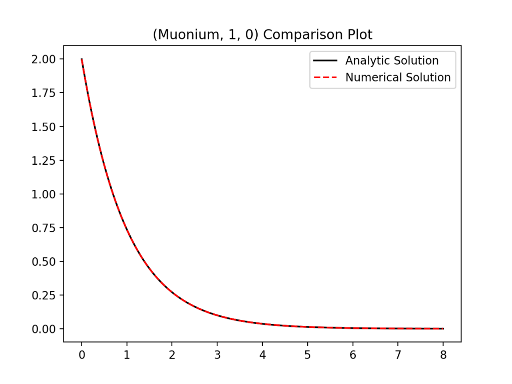
- we insert the form of N(r) in equation of u(r).
- Then, we train the network so as to minimize the error-function down to a quantity close enough to zero for all practical purposes.
- This is achieved by adjusting the biases (u_i) and weights (w_i).

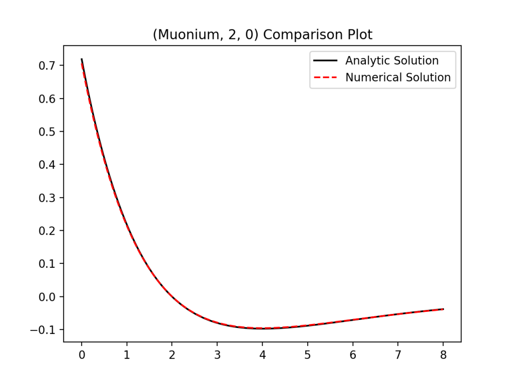
The energy of the corresponding atomic orbit is determined from the minimum energy-eigenfunction

The training in our method was performed using the BFGS and trust-constr algorithms as provided from the Python submodule SciPy.optimize

Comparison of analytical and numerical solution

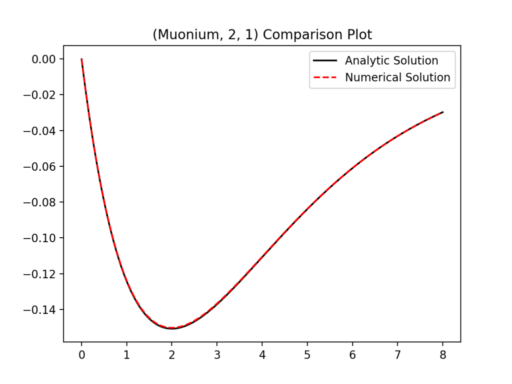
For $n = 1, 2, 3$ and $l = 0, \ldots, n-1$ the results are the following (Number of nodes: 10, Size of grid: 100) [axis: r/a_0, $R * a_0^{3/2}$]

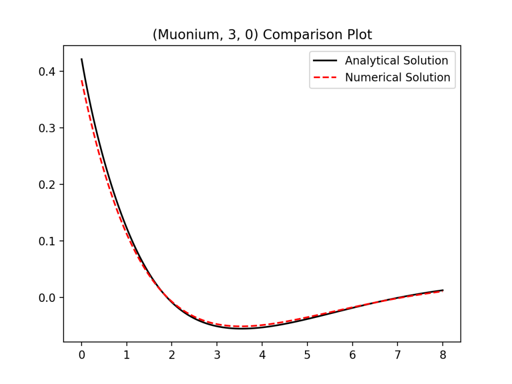




Comparison of analytical and numerical solution

Preliminary Results





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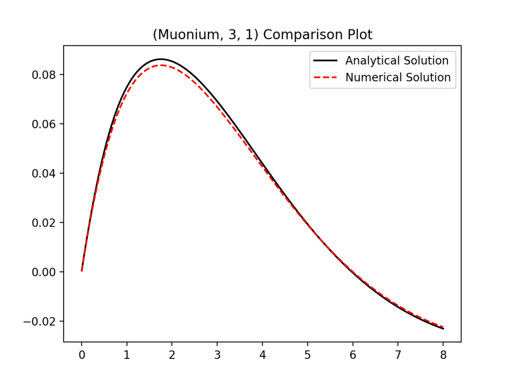

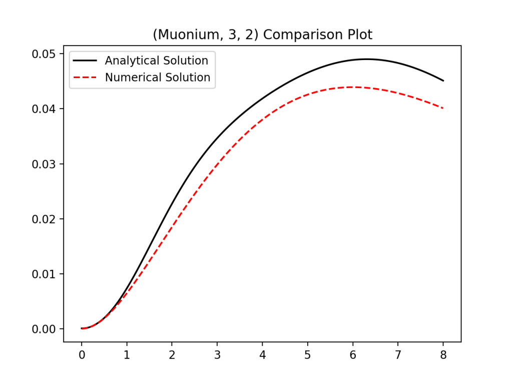

Dirac equation

Proceeding to the Dirac radial coupled equations system,

$$\frac{d}{dr}f(r) + \frac{k}{r}f(r) = \frac{1}{\hbar c}(\mu c^2 - E + V(r))g(r)$$

$$\frac{d}{dr}g(r) - \frac{k}{r}g(r) = \frac{1}{\hbar c}(\mu c^2 + E - V(r))f(r)$$

the respected error function is,

$$F_{err}^{D}(f,g) = \frac{\sum\left[\frac{df(r_i)}{dr} + \frac{k}{r_i}f(r_i) - \frac{\mu c^2 - E + V(r_i)}{\hbar c}g(r_i)\right]^2 + \sum\left[\frac{dg(r_i)}{dr} - \frac{k}{r_i}g(r_i) - \frac{\mu c^2 + E - V(r_i)}{\hbar c}f(r_i)\right]^2}{\int_0^\infty [g^2(r) + f^2(r)]dr}.$$

- We have presented an numerical method for solving the Schrödinger and the Dirac equation, which can include relativistic terms (Breit, Darwin, etc.)
- We assessed the effectiveness of the method by comparing the numerical solution with the analytic ones whenever possible (non-relativistic case, Schr. eq.)
- For the numerical solution we adopted an N.N. technique based on the minimization of the error function.
- We conclude that for small quantum numbers, the agreement is excellent even in the cases of using a small number of nodes, but for bigger ones a greater partition is required.
- The applied method is for the accurate description of exotic purely leptonic atoms for which extremely sensitive experiments all over the world provide relevant spectroscopi data.

Thank You!

Ioannina

Kastoria