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Development of a numerical solving software for the Dirac equation

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Introduction

In many physical problems, one needs to describe accurately the motion of bound leptons (e, μ, τ, etc.) in atomic orbits. Because this motion is relativistic, one must move from the Schrödinger equation and solve the Dirac equation in the field of the finite size nuclei. Moreover, for high Z values of the atomic nuclei, the motion of a muon, tau leptons, etc. is relativistic, and the small component f(r) of their wave functions is non-negligible.
As a result that component of the Dirac equation needs also to be calculated.
Here we present, the Dirac system of radial equations for hydrogen-like atoms is shown and a proposed numerical scheme based on neural networks is presented. Before that the (time-independent) Schrödinger equation since their solutions are similar.
The results obtained can be used for:

1. Nuclear size corrections to the energy levels of single-muon atoms
2. Accurate determination of the bound energy spectra in purely leptonic atoms: Muonium, true Muonium, etc.

The Radial equation

The Schrödinger Equation

Beginning with the radial equation for the Schrödinger equation,

$$\boxed{\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)\right)u(r)=Eu(r).}$$

where μ denotes the respected reduced mass of the system, given by

$$\mu=\frac{m_a m_b}{m_a+m_b}$$

where m_a and m_b denote the mass of particles a and b of the system respectively. The solutions of the equation assuming that $V(r)$ is the Coulomb potential of the form $-e^2/r$, where $e^2 = 1.4399764\ MeV\ fm$, denotes the elementary charge, is of the form

$$\boxed{u(r)=\sqrt{\left(\frac{2}{na_0}\right)^3\frac{(n-l-1)!}{2n(n+l)!}}e^{\frac{-r}{na_0}}\left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)}$$

where a_0 is the Bohr radius of the leptonic system and n, l are the quantum numbers.

The Dirac equation

As for the Dirac equation the respected radial equations in this case is the system,

Radial equations system

$$\frac{dg}{dr}+\frac{1+k}{r}g=\frac{1}{\hbar c}(E_0+E+V)f$$

$$\frac{df}{dr}+\frac{1-k}{r}f=\frac{1}{\hbar c}(E_0-E-V)g$$

where $E_0 = mc^2$ is the rest mass of the system.

This system of equations admits solutions of the form

Analytical Solutions

$$g(r)=\frac{(2\lambda)^{3/2}}{\Gamma(2\gamma+1)}\left[\frac{(1+\epsilon)\Gamma(2\gamma+1+n')}{4N(N-k)n'!}\right]^{1/2}(2\lambda r)^{\gamma-1}e^{-\lambda r}$$
$$[(N-k)F(-n',2\gamma+1,2\lambda r)-n'F(1-n',2\gamma+1,2\lambda r)]$$

$$f(r)=-\frac{(2\lambda)^{3/2}}{\Gamma(2\gamma+1)}\left[\frac{(1-\epsilon)\Gamma(2\gamma+1+n')}{4N(N-k)n'!}\right]^{1/2}(2\lambda r)^{\gamma-1}e^{-\lambda r}$$
$$[(N-k)F(-n',2\gamma+1,2\lambda r)+n'F(1-n',2\gamma+1,2\lambda r)]$$

where

$$\epsilon=\frac{E}{E_0},\quad \lambda=\frac{E_0}{\hbar c},\quad N=\frac{\alpha}{\sqrt{1-\epsilon^2}}$$

with $\alpha \approx 1/137$ denoting the fine structure constant. The energy E is given by

$$E=mc^2\left[1+\frac{\alpha^2}{\left(n-|k|+\sqrt{k^2-\alpha^2}\right)}\right]^{-1/2}.$$

Proposed Numerical Solution of the Dirac equation using N.N.

Let as assume first that u is a solution of the Schrödinger radial equation, if $r_1,\ldots,r_k > 0$, then u must also satisfy,

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

Now let as assume that u is a numerical solution of the form

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

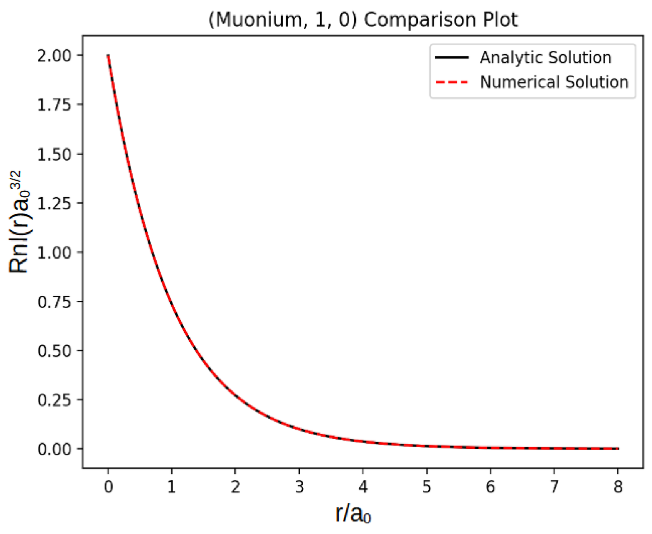
where

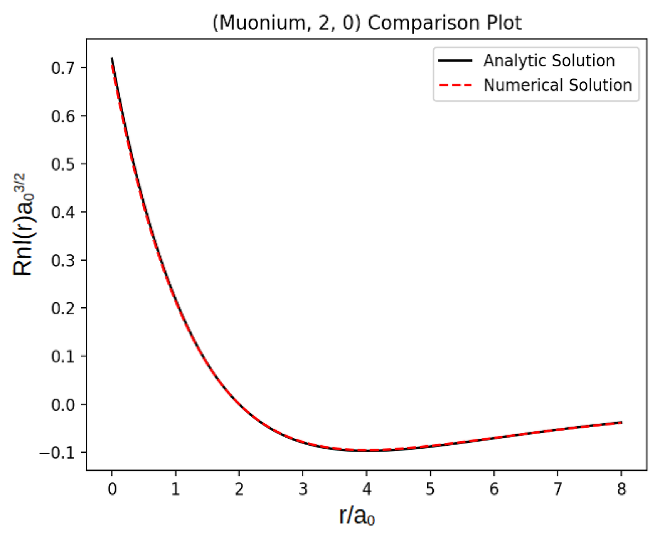
$$Nf(r,u,v,w)=\sum_{i=1}^{s}u_i f(v_i r+w_i)$$

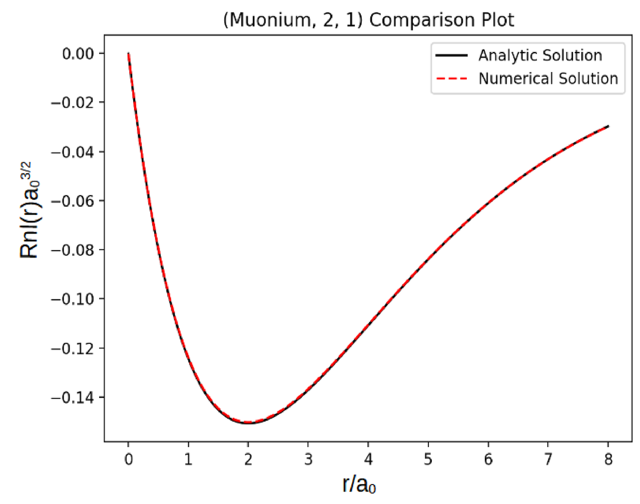
and f is the sigmoid function.
Then Nf is a 1-layer neural network with sigmoid activation functions. It should be noted here that the above parameterization was chosen so that $u(0) = 0$ and $u(r) \sim e^{-r}$.
Substituting u back to the radial equation, we obtain the error function,

$$\boxed{E_f(r,u,v,w)=\sum_{i=1}^{k}\left[\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r_i)\right)u(r_i)-Eu(r_i)\right]^2}.$$

The aim now is to minimize the above function for every $r > 0$, in the scale we need, i.e. to find u, v and w so that the error function is close or equal to zero. Utilizing the built-in Python methods, BFGS and trust-constr we obtain the following results.







For the Dirac equation, in the same vein as before, we first again formulate f and g as follows,

$$f(r)=re^{-k_f r}Nf(r,u_f,v_f,w_f)$$
$$g(r)=re^{-k_g r}Nf(r,u_g,v_g,w_g)$$

and the respected error function as,

Error function

$$E_f(r,u_g,v_g,w_g,u_f,v_f,w_f)=$$
$$\left[\frac{dg}{dr}+\frac{1+k}{r}g-\frac{1}{\hbar c}(E_0+E+V)f\right]^2$$
$$+\left[\frac{df}{dr}+\frac{1-k}{r}f-\frac{1}{\hbar c}(E_0-E-V)g\right]^2$$

As for the energy it can be obtained as follows,

Energy value

$$E=\frac{mc^2\int_0^\infty[g^2(r)+f^2(r)]dr+\int_0^\infty V(r)[g^2(r)-f^2(r)]dr}{\int_0^\infty[g^2(r)-f^2(r)]dr}.$$

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