Exploiting Dirac equations solution for exact integral calculations in processes of muonic atoms

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Abstract. Precise muon wave functions are calculated by solving the Dirac equations within a method based on modern neural networks and stochastic optimization techniques. The reduced radial wave functions (up and bottom) of a bound muon in muonic atoms are then given as linear combinations of the well behaved sigmoid functions. As concrete applications, the known muon-nucleus overlap integrals, which determine the structure and evolution of muonic atoms (two-body quantum systems bound together due to the fundamental electromagnetic interactions), may accurately be calculated. In this work, the muon-nucleus integrals for a set of nuclei including the $^{28}$Si and $^{64}$Zn entering the ordinary muon capture rates are exactly obtained through numerical integrations using Gauss integration algorithms.

1. Introduction

In modern physical problems, related to the structure and evolution of quantum systems, the evaluation of exact predictions for various physical observables is required [1, 2, 3]. These predictions are based on wave functions describing the states of the quantum system in question that come out of accurate solutions of specific type differential equations like the Schrödinger, the Dirac and the Klein-Gordon equations [1]. Because, usually, analytic solutions of such differential equations describing many body quantum systems are not possible, the application of advanced algorithms is required [4, 5, 6, 7].

Recently, a method for obtaining precise wave functions by solving the Dirac equations within neural networks and stochastic optimization techniques, has been derived [1]. Among the interesting applications of the respective algorithm (called DiracSolver), are the calculations of the up and bottom components of the radial wave functions for bound leptons, electron ($e^-$), muon ($\mu^-$) and tau ($\tau^-$), in the field of complex nuclei.

In the current research of physical sciences (atomic, molecular, nuclear physics, etc), the investigation of various processes taking place in muonic atoms possess prominent position. Well known such processes are, for example, the following: (i) The ordinary muon-capture by the nucleus (A,Z), A denoting the mass- and Z the atomic-number of the nucleus, and (ii) the
neutrinoless capture of a bound muon ($\mu_b^-$) in muonic atoms, known as muon-electron conversion. These processes are represented by the reactions

$$\mu_b^- + (A, Z) \rightarrow \nu_\mu + (A, Z - 1)^*, \quad (1)$$

$$\mu_b^- + (A, Z) \rightarrow e^- + (A, Z)^*. \quad (2)$$

Up to now, the evaluation of partial and total rates of such muonic processes was done by using approximate (mean) wave functions for the bound muons in nuclei \[2, 3, 9, 13\]. The purpose of the present work is to perform detailed calculations of the aforementioned muon-nucleus overlap integrals entering the partial and total rates of the ordinary muon capture. Specifically we concentrate on a set of prominent nuclear systems \[2, 3\] here focusing on the $^{28}\text{Si}$ and $^{64}\text{Zn}$ isotopes which are of current interest. Our final goal is to perform exact muon capture calculations for a list of currently interesting nuclear isotopes as $^{28}\text{Si}$, $^{32}\text{S}$, $^{48}\text{Ti}$, $^{56}\text{Fe}$, $^{66}\text{Zn}$ and $^{90}\text{Zr}$ studied recently by using a mean value of the ground state muon wave functions \[2, 3, 13\].

2. Formalism for the muon-nucleus overlap integrals

In the general case, the matrix elements $\mathcal{M}$ entering the expression of overlap integrals assuming non-relativistic muons are written as

$$\mathcal{M} = \langle f | \sum_{j=1}^{A} \Theta(j)e^{-i\mathbf{q} \cdot \mathbf{r}_j} \Phi_\mu(\mathbf{r}_j) | i \rangle, \quad (3)$$

where $|i\rangle$ the initial and $|f\rangle$ the final state of the daughter nucleus and $\Phi_\mu(\mathbf{r}_j)$ represents the radial part of the large (top) component of the muon spinor at the position of the $j^{th}$ target-nucleon. The functions $\Theta(j)$ depend on the specific (spin, isospin, etc. operator (function of the momentum transfer) and the studied process.

The methods of evaluating the $\mathcal{M}(q)$ can be classified in two-types according to how they treat the integrals of Eq. (3). The first determines them numerically using an exact muon wave function and the second uses an effective calculation of these integrals.

1). For process for which $|f\rangle = |i\rangle$, $\mathcal{M}_{gs}$ are written in terms of the ground state proton and neutron densities $\rho_p$ and $\rho_n$ as

$$\mathcal{M}_{gs} = \int [\rho_p(\mathbf{r}) \pm \rho_n(\mathbf{r})] e^{-i\mathbf{q} \cdot \mathbf{r}} \Phi_\mu(\mathbf{r}) d^3 \mathbf{r} \equiv \mathcal{F}_p \pm \mathcal{F}_n, \quad (4)$$

$$\mathcal{F}_{p,n}(q) = \int \rho_{p,n}(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}} \Phi_\mu(\mathbf{r}) d^3 \mathbf{r} \quad (5)$$

The proton (neutron) density $\rho_p$ ($\rho_n$) is normalized to the atomic number $Z$ (or to the neutron number $N$) of the participating nucleus in process (1).

Furthermore, for spherically symmetric systems the above integrals are simply written as

$$\mathcal{F}_{p,n}(q) = 4\pi \int j_0(qr)\Phi_\mu(r)\rho_{p,n}(r)r^2 dr, \quad (6)$$

where $j_0(x)$ represents the zero-order spherical Bessel function.

2). In the second case, the overlap integrals $\mathcal{M}$ are approximated by factorizing outside of the integrals of Eq. (3) a suitable average muon wave function $\langle \Phi_\mu \rangle$ as

$$\overline{\mathcal{M}}^{(\tau)}_\alpha = \langle \Phi_\mu \rangle \langle f | \sum_{j=1}^{A} \Theta(j)e^{-i\mathbf{q} \cdot \mathbf{r}_j} | i \rangle \equiv \langle \Phi_\mu \rangle \mathcal{M}, \quad (7)$$
where $M$ depends on the studied process and it is independent of the parameters of the muon. In the allowed muon capture process an approximation for the average value of $\langle \Phi_\mu (r) \rangle$ was used by many authors [2, 3]. It is given in terms of the effective charge $Z_{eff}$ of the nuclear system as

$$\langle \Phi_\mu \rangle ^2 = \frac{\int |\Phi_\mu (r)|^2 \rho (r) d^3r}{\int \rho (r) d^3r} = \frac{\alpha^3 m_\mu^3 Z_{eff}^2}{\pi Z}.$$  \hspace{1cm} (8)

($m_\mu$ is the muon rest mass). In previous estimations of the muon-capture rate [2, 3], the same expression (8) for $\langle \Phi_\mu \rangle$ was adopted for such calculations in various nuclear systems. In the present work, we calculate explicitly the integrals of Eq. (3) by first obtaining the muon wave function $\Phi_\mu (r)$ from the solution of the Dirac equation using the methods described in Ref. [1].

3. Muon wave functions from a stochastic optimization and neural network model

In a stochastic optimization model which uses neural networks, at first, a grid from $r = b$ is constructed. Beyond $r = b$, the wave function is practically vanishing (see below). We denote the grid by $r_i$, for $i = 1, 2, \cdots, n$. Then, the derivation of an appropriate error function to be minimized comes out of the differential Dirac equation which must hold at every point $r_i$ of the grid. This necessarily leads to the minimization of the error function [1].

Next, the approach involves the parametrization of the reduced radial wave functions $u_f(r)$, for the up component and $u_g(r)$, for the bottom component of the Dirac equation. The minimization of the error function is, in essence, an application of the least square fit. To this aim, for each of the $u_f(r)$ and $u_g(r)$, we use the parametrization

$$u(r) = re^{-kr}N(r, \vec{u}, \vec{w}, \vec{v}) , \quad k > 0 ,$$  \hspace{1cm} (9)

where $N(r, \vec{u}, \vec{w}, \vec{v})$ is a feed-forward artificial neural network with one hidden layer and one input unit ($r$) (for details see Ref. [1]). The biases are denoted by $\vec{u} = (u_1, u_2, \cdots, u_n)$ where $n$ is the number of hidden units. The weights to the hidden layers are denoted by $\vec{w} = (w_1, w_2, \cdots, w_n)$ and the weights to the output by $\vec{v} = (v_1, v_2, \cdots, v_n)$. The hidden layer units have sigmoid activations of the form $f(x) = (1 + e^{-x})^{-1}$. Specifically we have

$$N(r, \vec{u}, \vec{w}, \vec{v}) = \sum_{i=1}^{n} v_i f(w_i r + u_i) .$$  \hspace{1cm} (10)

To obtain the precise expressions for the reduced radial wave functions $u_f(r)$ and $u_g(r)$, we insert this form in Eq. (9). We then train the network so as to minimize the error function down to a quantity close enough to zero for all practical purposes, by adjusting the biases ($u_i$) and weights ($w_i$). The muon binding energy $\epsilon_b$ in the lowest atomic orbit is determined from the minimum energy, $E_{min} = \epsilon_b$, given by $\epsilon_b = E - m_\mu c^2$, with $E$ being the energy eigenvalue ($c$ denotes the speed of light). We note that the training in this method is performed by the DiracSolver software package [1], that has been proved to be both convenient and efficient.

3.1. Description of simulated annealing code

The method of simulated annealing, used in [1] for solving the Dirac equation, mimics the known annealing process to solve many optimization problems. This is based on a "temperature parameter" $T$ which controls the search process initially starting from a very high value and then is slowly "cooled" or lowered in every iteration. At each iteration a series of new points are generated. If the new point has a better error-function value it replaces the current point and the iteration counter is incremented. It is, however, possible to accept and move forward with a worse point, but the probability of doing so is directly dependent on the temperature $T$ (this
step, sometimes, helps identify a new search region in hope of finding a better minimum and protects the algorithm from being trapped in local minima). At this point we find it helpful for the reader to present a short description of simulated annealing algorithm as follows [1]:

1. Set $k = 0$, $T_0 > 0$. Sample $x_0$ as the initial point.
2. Set $N_{eps} > 0$, a positive integer.
3. Set $\epsilon > 0$, a small positive double precision value.
4. Set $r_T > 0$, $r_T < 1$, a positive double precision value.
5. For $i = 1, \ldots, N_{eps}$
   
   (a) Sample a point $y$
   
   (b) If $f(y) \leq f(x_k)$ then $x_{k+1} = y$
   
   (c) Else Set $x_{k+1} = y$ with probability $\min\left\{1, \exp\left(\frac{f(y)-f(x_k)}{T_k}\right)\right\}$

6. EndFor
7. Set $T_{k+1} = T_k r_T$
8. Set $k = k + 1$.
9. If $T_k \leq \epsilon$ terminate
10. Goto step 2.

It must also be mentioned that for large distances the matching of the wave functions to their asymptotic behavior was done as in Ref. [8]. For light muonic systems this matching was done at $r = b \approx 60-70$ fm and for heavy ones at $r = b \approx 40$ fm.

4. Results and discussion

The confidence level of using non-relativistic muon wave functions in muon physics calculations can be (to a large extent) estimated by solving, in addition to Schrödinger, the Dirac equations and obtaining the small component of the muon spinor as well. This is a Dirac-equation-based relativistic approach for the muon process. In the method of [1], the Dirac equation is solved in a more involved manner to that used for solving the Schrödinger equation in Ref. [8].

It is worth remarking that, the advantage of utilizing Eqs. (9)-(10) for the muon wave function, becomes more evident when one calculates the incoherent rate of a muonic process, where one has to face with a large number of numerical integrations corresponding to the final states $|f\rangle$ (in general a very large number). The computer-time needed to evaluate the muon-nucleus integrals when using the muon wave function described above is, sometimes, orders of magnitude shorter than that of other methods [10, 11, 12].

4.1. Solving Dirac equation for muonic atoms: Case of $^{28}$Si and $^{64}$Zn

In the context of the present method, we may investigate of the following effects:

(i) The consideration, in the process studied, of the muon as relativistic particle. This is estimated by comparing the radial Dirac wave functions for the muon with the Schrödinger one.

(ii) By comparing the exact results given by Schrödinger muon wave function with those obtained by using only the large (up) component of the Dirac wave function and neglecting the bottom component as done recently by the authors in [9].

(iii) The use of expression (7) for an approximate evaluation of the muon-nucleus integrals of Eq. (3). A mean value of the ground state muon wave functions was recently used for evaluating muon capture rates in the isotopes $^{28}$Si, $^{32}$S, $^{48}$Ti, $^{56}$Fe, $^{66}$Zn and $^{90}$Zr [2, 3, 13]. One of the main aims in the present calculations is to perform exact muon-capture calculations for the above systems in order to estimate this effect. As two concrete examples, in Fig. 1, we show the two components of the Dirac equation for a bound muon in the muonic atoms, bound two-body systems with the nucleus being the $^{28}$Si and the $^{64}$Zn nuclear isotope, respectively.
Figure 1: The two components of the Dirac equation: large for a bound muon in the muonic atom of $^{28}\text{Si}$ and $^{64}\text{Zn}$.

To check case (iii) above, we use the partial muon capture rate which takes the form [2, 3, 14]

$$\Lambda_{i\to f} = \frac{2G_\mu^2q_f^2}{2J_i+1} R_f \left[ \left| \langle J_f|\Phi_{1s}(\hat{M}_J - \hat{L}_J)|J_i\rangle \right|^2 + \left| \langle J_f|\Phi_{1s}(\hat{T}_f^j - \hat{T}_magn)|J_i\rangle \right|^2 \right]$$

(11)

(the various parameters and symbols of the latter equation are explained in Ref. [2, 3]). Such exact calculations are now in progress and the results will be published elsewhere.

5. Conclusions and future work

We have developed a method of direct calculation of the muon-nucleus integrals entering muon processes in muonic atoms. This method uses the precise muon wave functions obtained in the framework of neural network techniques and stochastic optimization in the form of a sum over few sigmoid functions.

We have, furthermore, exploited these muon wave functions, both in the Schrödinger and Dirac pictures, to test some approximations used in the past in muon capture processes. Due to experimental interest of this process in the near future we are going to extent these calculations in a list of prominent nuclear isotopes as $^{28}\text{Si}$, $^{32}\text{S}$, $^{48}\text{Ti}$, $^{56}\text{Fe}$, $^{66}\text{Zn}$ and $^{90}\text{Zr}$ studied recently.

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