We present a new open-source software for the integration of the radial Dirac equation developed specifically with muonic atoms in mind. The software, called mudirac, is written in C++ and can be used to predict frequencies and probabilities of the transitions between levels of the muonic atom. In this way, it provides an invaluable tool in helping with the interpretation of muonic X-ray spectra for elemental analysis. We introduce the details of the algorithms used by the software, show the interpretation of a few example spectra and discuss the more complex issues involved with predicting the intensities of the spectral lines. The software is available publicly at https://github.com/muon-spectroscopy-computational-project/mudirac.

1 | INTRODUCTION

Muonic atoms, in which one electron is replaced by the much heavier muon, have long been known and studied as an interesting laboratory for many kinds of exotic effects and insights in physics.\cite{1,2} The muon is a fundamental particle that can be created naturally when cosmic radiation bombards the Earth's atmosphere, or artificially in particle colliders. Muons are leptons, and comes as either negatively or positively charged, corresponding to the particle and its anti-particle. It has a spin $-1/2$ and a mass that is approximately 208 times that of an electron and thus one-ninth that of a proton. Thanks to this higher mass, a muon surrounding an atomic nucleus has orbitals much smaller than an electron, and thus interacts far more strongly with the nucleus, probing effects such as vacuum polarisation\cite{3} and the internal structure of the proton.\cite{4} More recently, interest in using muonic atoms for elemental analysis has arisen.\cite{5,6} There are currently five sources that can produce muons useful for investigating new and novel materials, namely TRIUMF (Canada), PSI (Switzerland), ISIS (UK), JPARC (Japan) and MUSIC (Japan). Muons are produced by having a beam of high-energy protons collide with a carbon target approximately 1 cm thick. The proton–proton collisions produce pions, which, in turn, are extracted based on their charge and focused into a beam. Negative pions decay in flight to produce muons, which are then implanted in the sample. These negative muons, after slowing down sufficiently to be captured by an atom, cascade down as they occupy lower and lower orbitals. The X-rays emitted during this cascade process are a very distinct elemental fingerprint and can be used to determine the sample's composition.

Used in this way, muons provide a very powerful probe that is non-destructive and can be tuned in depth by varying the momentum of the incident beam. This technique is especially useful when analysing archaeological artefacts, which could be damaged by any approach that required extracting a sample from them. Besides cultural heritage,\cite{7,8} this technique has been used for advanced manufacturing, battery materials, meteorites,\cite{9} biological samples,\cite{10,11} functional materials\cite{12} and imaging.\cite{13}

There are obvious analogies between elemental analysis with muons and X-ray fluorescence (XRF). The main
difference is in the mass of the probe particle, which results in the energy of the muonic X-rays being much greater than that of an X-ray emitted from fluorescence. In addition, as the momentum of the muon can be varied, muonic X-ray emission spectroscopy (μXES) is a depth-dependent probe and can result in elemental analysis below the surface, whereas generally XRF is a surface probe. The main drawback of μXES is that the data rates are much lower, so that at best elements in sub % concentrations can be detected, whereas XRF can measure trace elements.

While there exist tabulated databases of muonic atom X-ray frequencies\cite{14} and dedicated codes have been developed in the past to compute them,\cite{15} we still regarded it as useful to develop a new, modern code that could be used to aid with muon elemental analysis at ISIS. With this in mind, we have developed mudirac, an open-source C++ solver for the radial Dirac equation, designed specifically for computation of muonic X-ray spectra. Mudirac can compute most muonic atom transition energies up to precisions in the order of the keV, accounting for the effects of finite nuclear size, vacuum polarizability and electronic shielding, predicting both energies and transition probabilities for X-ray lines. This paper will provide an overview of the algorithms employed, a short documentation on how to use the software, and finally some tests and comparisons with reference sample spectra.

2 THEORY

2.1 The radial Dirac equation

The Dirac equation for a radial potential can be reduced to a pair of first-order one-dimensional differential Equations\cite{16-18}:

\[
\frac{d Q}{dr} = \frac{k}{r} Q + \left( mc - \frac{E - V(r)}{c} \right) P
\]

\[
\frac{d P}{dr} = -\frac{k}{r} P + \left( mc + \frac{E - V(r)}{c} \right) Q
\]

in which \( P \) and \( Q \) represent two components of the equation, with \( P \) being the “large” one when close to the non-relativistic regime. Here, \( m \) is the mass of the orbiting particle, or can be replaced by the effective mass, \( \mu = (1/m + 1/M)^{-1} \), including the effect of recoil from the nuclear mass \( M \) if one does not treat the nucleus as having infinite mass. In this equation all the following atomic units are used, so that \( e = \hbar = 1 \) and \( c = 1/\alpha \approx 137 \). \( k \) is a quantum number that can take on any positive or negative integer values (but not zero). In terms of the angular momentum and total angular momentum quantum numbers used in the Schrödinger equation, \( l \) and \( j \), we have that

\[
k = \begin{cases} 
-(l+1) & j = l+1/2 \\
l & j = l-1/2
\end{cases}
\]

The full three-dimensional wavefunction can then be reconstructed as follows:

\[
\langle r|\psi_{k\mu}\rangle = \begin{pmatrix} \frac{P_s(r)}{r} \langle \mathbf{r}|k\mu\rangle \\ \frac{Q_s(r)}{r} \langle \mathbf{r}|k\mu\rangle \end{pmatrix}
\]

where we make use of the spin spherical harmonics:

\[
|k\mu\rangle = \sum_{s=\pm 1/2} c\left(l, \frac{1}{2}; \mu - s, s\right) |l, \mu - s\rangle \Phi(s) \tag{4}
\]

with

\[
\langle \mathbf{r}|l, \mu - s\rangle = Y_{l\mu - s}(\mathbf{r}), \tag{5}
\]

\[
\Phi\left(\frac{1}{2}\right) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \Phi\left(-\frac{1}{2}\right) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{6}
\]

\( Y_{lm} \) being the usual spherical harmonics, and the Clebsch–Gordan coefficients

\[
c\left(l, \frac{1}{2}; \mu - s, s\right) = \begin{cases} 
-\text{sgn}(k) \sqrt{\frac{k + \frac{1}{2} - \mu}{2k + 1}} & s = \frac{1}{2} \\
\sqrt{\frac{k + \frac{1}{2} + \mu}{2k + 1}} & s = -\frac{1}{2}
\end{cases} \tag{7}
\]

as seen in\cite{16,19} and remembering Equation (2) for the relationship between \( k \) and \( l \).

Particular attention should also be paid to nodal theorems for this equation, as they are a useful guide when searching for solutions. The rule is that the large component of the wavefunction, \( P \), has always \( n - l - 1 \) nodes, while the \( Q \) component has \( n - l - 1 \) nodes if \( k < 0 \), and \( n - l \) nodes if \( k > 0 \).\cite{20,21}

2.2 Potential

The base potential used in Equation (1) is the Coulomb potential; however, it is important to note that this cannot be the traditional point charge Coulomb potential often used as a first approximation to solve atomic
potentials. In fact, especially for heavy atoms, muon states are so sensitive to the internal structure of the nucleus they have been historically among the first probes used to explore it.\[22,23\] The simplest way to account for the finite size of the nucleus is to treat it as a uniformly charged sphere of radius $R$:

$$V(r) = \begin{cases} -\frac{Z}{R} \left( \frac{3}{2} r^2 - \frac{1}{2} r^3 \right), & r \leq R \\ -\frac{Z}{r}, & r > R \end{cases}.$$ \hspace{1cm} (8)

The values for the radii of most isotopes of physical interest used in nuclear physics were extracted from the work by Angeli and Marinova.\[24\] It should be noted that the values tabulated in the paper are values for the root mean square radius, which means they need to be multiplied by $\sqrt{5}/3$ to get the equivalent radius of a uniformly charged sphere. For any isotope for which the radius is not known, we fall back on the empirical formula\[1\]:

$$R = 1.2A^{1/3} \text{fm} = 2.267 \cdot 10^{-5} A^{1/3},$$ \hspace{1cm} (9)

where the second version is in atomic units.

While sufficient to achieve satisfying accuracy for most cases, this finite sphere approximation still produces significant errors in some extreme circumstances, in particular transitions between the first two shells in heavy elements such as lead. In this case, a further increase in accuracy can be achieved by smoothing the charge distribution from a sphere with a sharp cut-off to a Fermi 2-term distribution\[25\]:

$$\rho(r) = \rho_0 \frac{1}{1 + e^{4\ln(3) - \frac{R_F}{r}}}.$$ \hspace{1cm} (10)

where $R_F$ and $\delta_F$ are two parameters corresponding roughly to the size of the nucleus and the thickness of its “skin,” the shell across which the density falls to zero. In particular, $R_F$ is connected to the corresponding uniform sphere radius $R$ for the same nucleus by

$$R_F = \left( R^2 - \frac{7}{3} \left( \frac{4\pi \delta_F}{4\ln(3)} \right)^2 \right)^{1/2}.$$ \hspace{1cm} (11)

for atoms where in atomic mass units $A \geq 5$, while for lighter nuclei, where the above formula would fail, we set

$$R_F = \left( 2.2291 \cdot 10^{-5} A^{1/3} - 0.90676 \cdot 10^{-5} \right),$$ \hspace{1cm} (12)

in atomic units. In following with Visscher and Dyall\[25\] we also take $\delta_F = 2.3 \text{ fm} = 4.3464 \cdot 10^{-5}$ for all nuclei. The charge distribution in Equation (10) does not produce a potential that can be described analytically; in this case, the Coulomb potential is computed by integrating instead of the differential equation

$$\frac{\partial}{\partial r} \left( r^2 \frac{\partial V}{\partial r} \right) = 4\pi r^2 \rho_{\text{bg}}(r),$$ \hspace{1cm} (13)

which comes by simple application of Gauss’s law in spherical coordinates. A way to integrate this equation numerically on a logarithmic grid is detailed in Section 3.4.

Two possible corrections to the Coulomb potential have been considered relevant for this software tool, as they have been shown to be largely the biggest contributions to transition energies, especially in heavy muonic atoms.\[1\] The first one is the so-called Uehling potential, representing the first-order contribution of vacuum polarisability to the interaction between the nucleus and the muon—in other words, the contribution of a Feynman diagram in which a photon exchange between muon and nucleus is mediated through an electron–positron pair production loop. This potential has a well-known form and can be written as

$$V_U(r) = -\frac{2\alpha Z}{3\pi r} \int_0^1 du \sqrt{1-u^2} \left[ \frac{1}{u} + \frac{1}{2} u \right] e^{-2\alpha r/u},$$ \hspace{1cm} (14)

for a point charge,\[26,27\] and

$$V_U^{\text{distr}}(r) = -\frac{2\alpha^2}{3r} \int_0^{\infty} dx \rho(x) \int_0^1 du \sqrt{1-u^2} \left[ \frac{1}{u} + \frac{1}{2} u \right] \left( e^{-2\alpha(r-x)/u} + e^{-2\alpha(r+x)/u} \right),$$ \hspace{1cm} (15)

for a generic charge distribution $\rho(r).$\[28\] For the specific case of a uniform spherical charge density,

$$\rho(r) = \begin{cases} \frac{3}{4\pi R_F^2} Z & r \leq R \\ 0 & r > R \end{cases}.$$ \hspace{1cm} (16)

the integral becomes

$$V_U^{\text{sphere}}(r) = -\frac{\alpha^2 Z}{2\pi r R_F^2} \int_0^r dx \int_0^1 du \sqrt{1-u^2} \left[ \frac{1}{u} + \frac{1}{2} u \right] \left( e^{-2\alpha(r-x)/u} + e^{-2\alpha(r+x)/u} \right).$$ \hspace{1cm} (17)
The integral in $x$ can be carried out if we consider the two distinct cases of $x < r$ and $x \geq r$. For the first case, we have

$$X < (r, u | R) = \int_0^R x \left( e^{-2c|r-x|/u} - e^{-2c(r+x)/u} \right) dx = e^{-2cr/u} \int_0^R x \left( e^{2cx/u} - e^{-2cx/u} \right) dx = e^{-2cr/u} \left[ e^{2cr/u} \left( \frac{Ru}{2c} - \frac{u^2}{4c^2} \right) + e^{-2cr/u} \left( \frac{Ru}{2c} + \frac{u^2}{4c^2} \right) \right],$$

while for the second case,

$$X > (r, u | R) = \int_0^R x \left( e^{-2c|r-x|/u} - e^{-2c(r+x)/u} \right) dx = \int_0^R x \left( e^{2cx/u} - e^{-2cx/u} \right) dx = -\frac{Ru}{2c} e^{-2cr/u} - \frac{u^2}{4c^2} \left( e^{-2cr/u} - 1 \right).$$

It then follows that the full term can be expressed as

$$V_{U}^{(\text{sphere})} (r) = -\frac{\alpha^2 Z}{2\pi R^3} \int_0^1 du \sqrt{1-u^2} \left( 1 + \frac{1}{2} u^2 \right) \left[ X < (r, u | \min(r,R)) + X > (r, u | R) - X > (r, u | \min(r,R)) \right]$$

which is the expression used for the Uehling potential in the software. The integration over $u$ is left to be carried out numerically.

The second correction adopted is the contribution of an electronic background charge. The way the charge distribution is computed in this case is described in Section 3.3; the differential equation to integrate is given in Equation (13).

### 2.3 Transition probabilities

To compute the transition probabilities between two states in the presence of an electromagnetic field, we need to compute the dipole matrix element between them. For spontaneous emission between two states, $a$ and $b$, in atomic units, we have,

$$W_{ab} = \frac{4E_{ab}}{3c} \left| \langle a | \alpha | j_0(kr) | b \rangle \right|^2,$$

with $E_{ab}$ transition energy, the wave vector has magnitude $k = E_{ab}/c$, and $\alpha$ is the vector of Dirac matrices $\alpha_y, \alpha_z$. If we consider the wavefunction written as seen in Equation (3), then it follows that each individual matrix element can be written as

$$\langle a | \alpha | j_0(kr) | b \rangle = i \langle k_a | \sigma_i | k_b \rangle \int_0^\infty j_0(kr) P_0 Q_0 dr - \int \langle -k_a | \sigma_i | k_b \rangle \int_0^\infty j_0(kr) P_0 Q_0 dr,$$

with $\sigma_i$ being the Pauli matrices, keeping in mind that

$$\alpha_i = \left[ \begin{array}{cc} 0 & \sigma_i \\ -\sigma_i & 0 \end{array} \right].$$

It should be recalled that in Equation (22) the minus sign appears because the part in the bracket is the adjoint, and not merely the complex conjugate, of the wavefunction. Now, keeping in mind Equation (4) and (5), and shortening the Clebsch–Gordan symbols seen in Equation (7) as $c_{k\mu} = c(l, \frac{1}{2}; \mu - s, s)$, we have

$$|k\mu\rangle = \left[ \begin{array}{c} c_{k\mu}^{1/2} Y_{l\mu - 1/2} \\ c_{k\mu}^{-1/2} Y_{l\mu + 1/2} \end{array} \right]$$

and therefore,

$$\langle k'\mu' | \sigma_\alpha | k\mu \rangle = \left( c_{k'\mu'}^{1/2} c_{k\mu}^{1/2} - c_{k'\mu'}^{-1/2} c_{k\mu}^{-1/2} \right) \delta_{l\mu} \delta_{l\mu'},$$

$$\langle k'\mu' | \sigma_+ | k\mu \rangle = c_{k'\mu'}^{1/2} c_{k\mu}^{-1/2} \delta_{l\mu} \delta_{l\mu'} + 1,$$

$$\langle k'\mu' | \sigma_- | k\mu \rangle = c_{k'\mu'}^{-1/2} c_{k\mu}^{1/2} \delta_{l\mu} \delta_{l\mu'} - 1.$$

If we also set for brevity

$$J_{ab} = \int_0^\infty j_0(kr) P_0 Q_0 dr,$$

and we consider that if to a certain $k$ corresponds an $l$, then to $-k$ corresponds $l - \text{sgn}(k)$, then Equation (22) reduces to

$$\langle a | \alpha | j_0(kr) | b \rangle = i \left[ \begin{array}{c} c_{l\mu}^{1/2} c_{-k\mu}^{1/2} \delta_{l\mu + 1} + c_{-k\mu}^{1/2} c_{l\mu}^{1/2} \delta_{l\mu} + 1 \rangle \delta_{l\mu} \delta_{l\mu'} \right] \delta_{l\mu} \delta_{l\mu'} J_{ab} - \left[ c_{l\mu}^{-1/2} c_{-k\mu}^{-1/2} \delta_{l\mu} + 1 + c_{-k\mu}^{-1/2} c_{l\mu}^{-1/2} \delta_{l\mu} + 1 \rangle \delta_{l\mu} \delta_{l\mu'} \right] J_{ab}.$$
\( \langle a | \alpha \beta (kr) | b \rangle = -\left( e^{-\frac{1}{2}c_{k(\mu \lambda)}^{-1/2}\delta_{\mu \nu} + 1} - e^{-\frac{1}{2}c_{k(\mu \lambda)}^{-1/2}\delta_{\mu \nu} + 1} \right) \delta_{\mu \nu} - \delta_{\mu \nu} \text{sgn}(\lambda) J_{ab} \).

\( \langle a | \alpha \beta (kr) | b \rangle = i \left( e^{-\frac{1}{2}c_{k(\mu \lambda)}^{-1/2}\delta_{\mu \nu} + 1} - e^{-\frac{1}{2}c_{k(\mu \lambda)}^{-1/2}\delta_{\mu \nu} + 1} \right) \delta_{\mu \nu} - \delta_{\mu \nu} \text{sgn}(\lambda) J_{ab} \).

(30)

\( \langle a | \alpha \beta (kr) | b \rangle = \frac{1}{2j_a + 1} \sum_{\mu} \sum_{\rho} W_{ab} \)  \( \sum \) over all possible states that are being integrated. In particular, by default we have

\( r_0 = \max \left( \frac{1}{Z \mu}, R \right) \),

(35)

namely \( r_0 \) is chosen as the maximum between the expected radius of an ideal Schrödinger 1 \( s \) orbital for a system with nuclear charge \( Z \) and reduced mass \( \mu \) and the finite radius of the nucleus.

The boundary conditions are found by solving Equation (1) analytically for the \( r \to 0 \) and \( r \to \infty \) limits. For a value of the energy \( E \), defining \( K = \sqrt{m^2 c^2 - E^2 / c^2} \), we find at infinity\(^{[18]} \):

\[ P(r) \approx e^{-Kr} \]  \( \text{(36)} \)

\[ Q(r) \approx -\frac{K}{mc + E/c} P(r). \]  \( \text{(37)} \)

At zero the situation is more complex, and differs depending whether we are considering a finite or point-size nucleus. For a point-size nucleus we have\(^{[30]} \):

\[ P(r) \approx r^\gamma \]  \( \text{(38)} \)

\[ Q(r) \approx -\frac{Z}{c(\gamma - k)} P(r) \]  \( \text{(39)} \)

with \( \gamma = \sqrt{k^2 - Z^2 c^2} \), while for a finite-size nucleus, we have for \( k < 0 \)

\[ P(r) \approx r^{-k} \]  \( \text{(40)} \)

\[ Q(r) \approx \frac{3Z}{2cR(-2k + 1)} r^{-k + 1} \]  \( \text{(41)} \)

and for \( k > 0 \)

\[ P(r) \approx r^{k + 2} \]  \( \text{(42)} \)

\[ Q(r) \approx \frac{2cR(2k + 1)}{3Z} r^{k + 1}. \]  \( \text{(43)} \)

### 3 | ALGORITHMS AND IMPLEMENTATION

#### 3.1 | Grid and boundary values

All calculations in mudirac make use of a logarithmic radial grid, so that \( r(x) = r_0 e^x \). In this way, the radial Dirac equation becomes

\[ \frac{\partial Q}{\partial x} = kQ + r(x) \left( mc - \frac{E - V(x)}{c} \right) P \]  \( \text{(33)} \)

\[ \frac{\partial P}{\partial x} = -kP + r(x) \left( mc + \frac{E - V(x)}{c} \right) Q. \]  \( \text{(34)} \)

Grid parameters are chosen case-by-case based on the parameters of the atom and the quantum numbers and energy of the state that is being integrated. In particular, by default we have

The radial Dirac equation is solved by a shooting method, integrating each step with a fourth-order Runge–Kutta (RK4) algorithm\(^{[31]} \) When using a shooting method to
integrate a boundary value problem, one applies the following iterative process

1. Start with a trial value for the eigenvalue, $E$;
2. Integrate the equation forward from zero and backwards from infinity, using that trial value, meeting halfway at the turning point (namely the point $r_t$ such that $V[r_t] = E$);
3. Compute an error based on how well the left and right solutions match at $r_t$;
4. Choose a new value of $E$ to minimize the error and repeat from step 2 until a certain tolerance is reached.

The important thing to decide is how to evaluate the matching described in step 3, and then how to optimise the energy. One might be tempted to simply look at how the values of the forward- and backward-integrated functions match at the turning point, for example, the values of the forward- and backward-integrated functions at $r_t$, but that would be a mistake. The functions at this point cannot be normalised, and so they are always known up to a constant term. Since this constant will be likely different between left and right integration (as it depends only on the boundary conditions), any absolute comparison is meaningless. Instead, it makes sense to consider the error

$$\delta y = y_f - y_b = \left. \frac{Q}{P_f} \right|_r - \left. \frac{Q}{P_b} \right|_r$$

(44)

that only depends on the ratio of $Q$ and $P$. When $E$ is an eigenvalue of the Dirac equation, namely when a solution has been found, we expect $\delta y = 0$; more in general, we expect we can find this energy by applying a steepest descent search and using the derivative of the error in the energy

$$\frac{\partial (\delta y)}{\partial E} = \frac{\partial y_f}{\partial E} - \frac{\partial y_b}{\partial E} = \zeta_f - \zeta_b$$

(45)

to minimize it. Now, making use of Equation (1), we find that we can write a differential equation for $y$

$$y' = 2 \frac{k}{r} y - g + y^2 + g$$

(46)

where the apices indicate differentiation in $r$ and we defined for convenience

$$g_\pm = \left( mc \pm \frac{E - V}{c} \right).$$

(47)

Differentiating in $E$ then we obtain

$$\zeta' = 2 \left( \frac{k}{r} - g + y \right) \zeta - \frac{1}{c} (y^2 + 1)$$

(48)

(remember that $\partial g_+/\partial E = -\partial g_-/\partial E = 1/c$). This differential equation can be easily integrated once we have a tentative $Q$ and $P$. The boundary conditions are found by differentiating the ones for $Q$ and $P$ and are

$$\zeta(r) \approx 0 \quad r \to 0$$

(49)

$$\zeta(r) \approx \frac{E}{c K g_+^2} + \frac{K}{c g_+} \quad r \to \infty.$$  

(50)

Integrating $\zeta$ forwards and backwards from the two extremes of the grid, we can then apply Equation (45) and use it to minimise the energy. The only problem is that $y$ has singularities in the poles of $P$, which causes practical difficulties in the integration of $\zeta$. This is easily fixed though if we consider an equation complementary to Equation (48), namely

$$\eta = \frac{\partial}{\partial E} \left( \frac{1}{y} \right) = -\frac{1}{y^2} \zeta$$

(51)

$$\eta' = -2 \left( \frac{k}{r} + g - \frac{1}{y} \right) \eta + \frac{1}{c} \left( \frac{1}{y^2} + 1 \right)$$

(52)

which can be integrated in all those parts of the domain in which $y$ grows too big. Performing a Runge–Kutta integration alternating between the two as needed, it is possible to estimate $\zeta_f - \zeta_b$ and thus converge the energy to an eigenvalue. From Equations (44) and (45) one can find that

$$\delta E \approx \delta y \frac{\partial E}{\partial (\delta y)} = \frac{y_f - y_b}{\zeta_f - \zeta_b}$$

(53)

Figure 1 shows an example of the results produced by this algorithm. For a muonic hydrogen atom and a range of initial energy guesses $E_0$, it shows what the algorithm predicts as the converged energy, $E_0 - \delta E$. If the linear approximation was correct, which of course tends to be true only when $E_0$ is close to an eigenvalue of the equation, then the figure would only show plateaus, with sudden jumps when the energy guess causes a new node to appear in the wavefunction, thus entering in the convergence basin of a different eigenvalue. These ideal plateaus, based on converged calculated energies and the number of nodes detected in the wavefunction, are
shown as a solid line in Figure 1. The curve for \( E_0 - \delta E \) appears instead as an approximation to it, but one can see how in practice a series of updates \( E_0' = E_0 - \delta E \) does generally converge quickly to the appropriate eigenvalue. However, convergence tends to get more difficult when considering higher energy levels, where the gaps between successive shells shrink.

In practice, when searching for a given state, one cannot be sure of what the best \( E_0 \) to start with is. An intuitive initial guess is the corresponding eigen energy for the hydrogen-like, Coulomb atom with a point nuclear charge\(^{[32]}\):

\[
E_{nj}^{(ideal)} = \mu c^2 \left( 1 + \frac{Z\alpha}{n - |k| + \sqrt{k^2 - Z^2/2}} \right)^2, \quad (54)
\]

with \( \mu \) as the effective mass of the system, and \( k \) as the quantum number defined in Equation (2). However, especially for \( Z \gg 1 \) and low \( n \), these energies can be very far from the real ones, once all corrections are taken into account. For these reasons, various considerations are in practice taken into account when seeking to converge a state with a given \( n \) and \( k \) in mudirac:

- The energy is taken to be bounded above by the rest mass, \( E_{nj} < \mu c^2 \), the requirement for the state to be bound;
- The energy is taken to be bounded below by the maximum between the value of the potential for \( r = 0 \) (if finite) and twice the ideal binding energy for the same atom, \( E_{nj} > \max \left( V(0) + \mu c^2, 2E_{1,-1}^{(ideal)} - \mu c^2 \right) \). This is an empirical condition but has been seen to work well across the periodic table and is a way to avoid energies that are too small or drift in the positron branch of the Dirac’s equation solutions;
- If any other states with the same \( k \) but different \( n \) have been calculated during the same run, their energies will be used appropriately as additional lower or upper bounds.

The ideal hydrogen-like energy is used as a starting value only if it falls within the bounds so defined; if it does not, then the middle point between minimum and maximum energy is used. The final converged state is then checked using the nodal theorems mentioned in Section 2.1. If, regardless of these precautions, the final state does not have the desired \( n \), it is still stored and its energy is used to determine the boundaries of the starting energy for the next iteration. This leads to eventually starting in the right basin, and thus finding the desired energy, in a few cycles.

### 3.3 Electronic background charge

While, in general, the higher mass of the muon means its orbitals are much smaller than the electronic ones, and thus the contribution of the repulsion from electrons is negligible, there can be some overlap between some of the higher muonic orbitals and some of the lower electronic ones, which introduce a small correction to the energy. A full treatment of this correction would require solving the many-body problem for both the muon and
all the electrons orbiting the atom, and at the moment has been considered unnecessarily complex for the scope of this software. Instead, the approach described by Tauscher et al.[33] has been used here.

The scheme fills iteratively the electronic shells of the atom using the following rules:

1. The shell with \( n = 1 \) is treated as seeing a nucleus of charge \( Z - 1 \), to account for the shielding caused by the muon;
2. Each successive shell is treated as seeing a nucleus of charge \( Z - 1 - q \), with \( q \) as the total number of electrons placed in lower shells.

The orbitals used are the standard hydrogen-like solutions of the Dirac Equation.[32] The total background electronic density is then obtained as the sum of the individual density contributions from the radial parts of each of the filled orbitals. The exact density is calculated by using a user-defined electronic configuration.

### 3.4 Potential from a background charge

In order to compute the contribution to the potential of an arbitrary background charge, such as the electronic one, as well as the Fermi 2-term nuclear charge distributions, one needs to integrate Equation (13). Let us assume the general case of a background charge \( \rho(r) \) defined between the two limits \( R_{\text{in}} \) and \( R_{\text{out}} \). On a logarithmic grid, the equation becomes

\[
\frac{\partial^2 V}{\partial x^2} + \frac{\partial V}{\partial x} = 4\pi r^2 \rho(r). \tag{55}
\]

This equation cannot be integrated with the Numerov method that is most often used for second-order differential equations due to the presence of a first-order term. Instead, a third-order scheme was used for making use of the following finite differentiation approximations:

\[
\frac{\partial V}{\partial x} \bigg|_{i} \approx \frac{1}{h} \left( \frac{11}{6} V_{i-3} - 3V_{i-1} + \frac{3}{2} V_{i-2} - \frac{1}{3} V_{i-3} \right) \tag{56}
\]

\[
\frac{\partial^2 V}{\partial x^2} \bigg|_{i} \approx \frac{1}{h^2} (2V_{i} - 5V_{i-1} + 4V_{i-2} - V_{i-3}), \tag{57}
\]

setting the first three points of \( V \) with an approximation of constant charge for \( r < R_{\text{in}} \) and shooting outwards for all the following ones. In general, the potential can be constructed piecewise at all values of \( r \) as follows:

\[
V_{\text{bkg}}(r) = \begin{cases} 
-\frac{Q}{r} & r > R_{\text{out}} \\
V_{\text{grid}}(r) - V_{\text{grid}}(R_{\text{out}}) - \frac{Q}{R_{\text{out}}} & R_{\text{out}} \geq r > R_{\text{in}} \\
\frac{2}{3} \pi r^2 \rho(R_{\text{in}}) - V_{\text{grid}}(R_{\text{out}}) - \frac{Q}{R_{\text{out}}} & r \leq R_{\text{in}}
\end{cases}
\]

with \( V_{\text{grid}} \) the potential integrated on the area of the grid in which \( \rho \) is explicitly defined, and the convention \( V_{\text{bkg}}(r) = 0 \) when \( r \to \infty \).

### 4 SOFTWARE DETAILS

Mudirac has been written to comply with the C++ 11 ISO standard.[34] It makes use of the libraries Catch, for testing, and Aixlog, for logging, which are included with the distribution. It is compiled into an executable that can be run as follows:

```bash
$> mudirac input.in
```

with the input file input.in (the name is arbitrary) containing all necessary parameters to determine the calculation. These include the atom type, the terms to include in the potential and which spectral lines should be calculated. A list of all possible keywords with their meaning and default values is included in the repository, in the file docs/Keywords.pdf.

The software produces the following output files:

- a .log and an .err file, containing regular logging of the program’s operation and any errors/exceptions thrown during the run. The amount of information in the log can be changed by setting a verbosity parameter in the input file;
- a .xr.out file containing a full report of the energy (in eV) and transition probabilities (in s\(^{-1}\)) for each requested spectral line, and excluding any lines for which calculations did not succeed or which were found to be forbidden transitions;
- optionally, a .spec.dat file containing a final simulated spectrum including all lines convoluted with Gaussian functions and with intensities proportional to their transition probability;
- optionally, a series of \(<\text{name}>\).out state files containing potential, \( P \) and \( Q \) components of the wavefunction for each computed state. The state names use the standard IUPAC X-ray spectroscopy convention[35];
- optionally, a series of \(<\text{name1}>. <\text{name2}>.tmat.out files containing the details of the transition matrix between two given levels, namely the transition rates
between each of their respective degenerate states of different $m_f$.

Atomic units are used inside the code and for most input parameters (either energy or masses). The only exception are parameters for the writing of .spec.dat files, in which those that have units of an energy must be set in electron volts.

Mudirac is an open-source software; it has been released publicly under the MIT License, and is available at the URL https://github.com/muon-spectroscopy-computational-project/mudirac as part of the tools produced by the Muon Spectroscopy Computational Project.

5 | EXAMPLES AND TESTS

5.1 | Hydrogen lines

While mudirac was designed with muons in mind, it is possible to set the mass of the particle to arbitrary values, so solving for electronic atoms is not a problem. As a first test of the functionality of mudirac’s solver, here we present the computed relativistic transition energies and probabilities for the hydrogen atom, compared to the well-known and tabulated experimental values in the NIST Atomic Spectra Database. Hydrogen constitutes the simplest possible model to run tests on: data for heavier atoms usually include the effect of additional electrons, and the availability of transition rate values makes it possible to evaluate the accuracy in computing these quantities too, for which experimental data are not available for muonic atoms.

Calculations with mudirac were run using a finite-size nuclear model and the Uehling potential correction on. The lines are labelled, the results are shown in Table 1 and show excellent agreement on both transition energies and probabilities.

5.2 | Muonic atom lines

Here we present a few examples of comparisons of spectral lines for muonic atoms to values reported in the literature, in particular in Borie and Rinker,[1] Kessler et al,[40] and Nelms et al,[41] and the spectra from the database presented in Zinatulina et al.[14] For the values found in Borie and Rinker[1], a reference computed value is available, besides the experimental one. These computed values are extremely accurate, including also field theory effects beyond the Uehling potential, thus it is not surprising that the mudirac computed values differ slightly. Values from the other sources are all experimental. The comparisons can be seen in Table 2.

Most computed energies fall within 1–2 keV of the experimental value. In Table 3, we break down the contributions to the final energy for all Pb lines by repeating the calculation adding effects one by one (in order: uniform spherical charged nucleus, Fermi 2-term charge distribution, Uehling correction and electronic screening) in order to analyse which are the most relevant to the final energy. The starkest difference between lines can be seen in the finite-size correction, which is in the eV range for N–O lines but goes up to 10 MeV for the K-L lines, as it is to be expected from these states having a much more significant overlap with the atomic nucleus. It must also be noted that there is a significant effect of around 50 keV introduced just by going from a uniform sphere model to a Fermi 2-term charge distribution for the nucleus. The electronic screening is the only correction that is bigger for N–O lines, since these overlap more with electronic orbitals, but it never goes above 0.1 keV.

### Table 1

| Line   | $E$ (eV) | $E_{NIST}$ (eV) | $A$ (s$^{-1}$) | $A_{NIST}$ (s$^{-1}$) | References                  |
|--------|----------|-----------------|----------------|------------------------|------------------------------|
| K1-L2  | 10.19884 | 10.19886        | 6.2649e+08     | 6.2649e+08             | Sansonetti et al[36] and Baker[37] |
| K1-L3  | 10.19889 | 10.19891        | 6.2648e+08     | 6.2648e+08             | Sansonetti et al[36] and Baker[37] |
| L1-M2  | 1.88869  | 1.88869         | 2.2449e+07     | 2.2449e+07             | Baker[37] and Zhao et al.[38] |
| L1-M3  | 1.88870  | 1.88871         | 2.2448e+07     | 2.2448e+07             | Baker[37] and Zhao et al.[38] |
| L3-M4  | 1.88866  | 1.88867         | 1.0775e+07     | 1.0775e+07             | Baker[37]                    |
| L3-M5  | 1.88866  | 1.88867         | 6.4651e+07     | 6.4651e+07             | Baker[37] and Hänsch et al.[39] |
| M1-N2  | 0.66104  | 0.66104         | 3.0652e+06     | 3.0652e+06             | Baker[37]                    |
| M1-N3  | 0.66104  | 0.66105         | 3.0650e+06     | 3.0650e+06             | Baker[37]                    |

Note: Last column contains the papers from which the values were originally taken.
The Uehling correction is around 30 keV for K-L lines, and much lower, albeit not insignificant, for N—O ones.

5.3 | Isotope effect

It has been shown\cite{42} that muonic X-ray analysis is also a good way to discern between isotopes of the same element, thanks to the effect of finite nuclear size and mass. Here we show the prediction made by mudirac for $^{204}$Pb, $^{206}$Pb, $^{207}$Pb and $^{208}$Pb, using as reference experimental data from the literature.\cite{40} Figures 2–4 show the predicted energies for the K1-L2, K1-L3 and L3-M5 transitions, respectively, for various isotopes of lead, compared to the known experimental values. The calculations were performed using a finite nuclear size, Uehling correction and electron screening as shown in Table 2. As it can be seen, the isotope effect is captured very well, with errors that are approximately constant across the various atomic weights, especially in the K-L transitions.

5.4 | Spectra comparisons

Finally, we consider a few example experimental spectra and compare them with mudirac computed results. The experimental spectra presented in this paper have utilised the ISIS pulsed neutron and muon source\cite{43} and in particular were acquired on the RIKEN-RAL beamlines\cite{44,45} with the RIKEN Port 4 instrument. The experimental set-up is shown in Figure 5. The muons, with the correct momentum, are emitted from the beam-pipe in the top centre of the figure. The sample is mounted in the centre. Surrounding the sample are four detectors in a cross configuration. In the most common current set-up, these are four high purity germanium detectors, with varying efficiencies and resolution. In general, the detectors can be classified into two groups, low energy (30–1000 keV) and high energy (100–8000 keV). However, if transition of low energies is of particular interest then a germanium detector can be replaced with a silicon detector, with an energy range of (5–200 keV). This allows the set-up to be optimised for the problem at hand.

The spectra shown here come in multiple bin widths, ranging from 2 to 0.5 keV between each point. The samples are pure elemental standards or metal alloys. For these experiments, the beam’s momentum was set in the range of 30–40 MeV/c. All calculations used for the simulated spectra include a Uehling correction and the standard electronic configuration for the element with $Z - 1$.

### Table 2
Computed and experimental energies in keV for various muonic atom lines

| Line        | Mudirac | Computed | Experimental |
|-------------|---------|----------|--------------|
| $^{16}$O, N6-O8 | 4.0224  |          | 4.0243\cite{41} |
| $^{16}$O, N7-O8 | 4.0216  |          | 4.0227\cite{41} |
| $^{16}$O, N7-O9 | 4.0218  |          | 4.0237\cite{41} |
| $^{24}$Mg, L2-M4 | 56.389  | 56.392\cite{11} | 56.392\cite{11} |
| $^{24}$Mg, L3-M5 | 56.214  | 56.216\cite{11} | 56.216\cite{11} |
| $^{204}$Fe, K1-L3 | 1.256.89 |          | 1.257.9\cite{14} |
| $^{206}$Fe, K1-M3 | 1.522.1  |          | 1.523.5\cite{14} |
| $^{206}$Fe, K1-N3 | 1.614.94 |          | 1.616.7\cite{14} |
| $^{105}$Sn, M4-N6 | 349.964  | 349.986\cite{11} | 349.975\cite{11} |
| $^{105}$Sn, M5-N7 | 345.252  | 345.256\cite{11} | 345.254\cite{11} |
| $^{204}$Pb, N6-O8 | 437.757  | 437.749\cite{11} | 437.749\cite{11} |
| $^{204}$Pb, N7-O9 | 431.359  | 431.336\cite{11} | 431.328\cite{11} |
| $^{204}$Pb, K1-L2 | 5.779.1  |          | 5.777.9\cite{40} |
| $^{204}$Pb, K1-L2 | 5.779.1  |          | 5.776.8\cite{14} |
| $^{204}$Pb, K1-L3 | 5.963.81 |          | 5.962.7\cite{40} |
| $^{204}$Pb, K1-L3 | 5.963.81 |          | 5.961.9\cite{14} |

**Note:** Energies computed with mudirac make use of a Fermi 2-term charge distribution for the nucleus, Uehling correction to the potential and an electronic background charge using the configuration of the atom with $Z - 1$ (so, for example, the configuration for $^{24}$Mg is that of neutral Na). Please note that the values from Zinatulina et al.\cite{14} are manually extracted from images of spectra and thus may be less accurate than the others.

### Table 3
Breakdown by contribution of the energy in keV for various lines in muonic lead

| Line        | $E_{\text{point}}$ | $dE_S$ | $dE_{F2}$ | $dE_U$ | $dE_e$ | $E_{\text{full}}$ |
|-------------|---------------------|--------|-----------|--------|--------|------------------|
| $^{204}$Pb, N6-O8 | 435.66              | -0.01  | 0.00      | 2.19   | -0.09  | 437.76           |
| $^{204}$Pb, N7-O9 | 429.34              | -0.00  | 0.00      | 2.10   | -0.09  | 431.36           |
| $^{204}$Pb, K1-L2 | 15,606.90           | -9,912.16 | 50.05   | 34.28  | -0.01  | 5,779.06         |
| $^{204}$Pb, K1-L3 | 16,155.10           | -10,279.74 | 51.66  | 36.80  | -0.01  | 5,963.81         |

**Note:** The contributions are the ideal point-like Coulomb potential energy ($E_{\text{point}}$), the contribution from including a uniform charged sphere nucleus ($dE_S$), the further refinement from using a Fermi 2-term charge distribution ($dE_{F2}$), the Uehling potential ($dE_U$) and finally the electronic screening ($dE_e$). The last column shows the final energy, $E_{\text{full}}$. 

---

\[42\] Zinatulina et al. \[14\]
as for the previous calculations. Simulated spectra have been generated simply by using a Gaussian broadening of 1 keV. Energies are in keV, and intensities are arbitrary units.

Figure 6 shows a comparison for the spectrum of aluminium, up to 450 keV. The experimental spectrum has a bin width of 0.5 keV. The computed one includes all lines involving states up to the O shell \((n = 5)\). One thing that can be noticed is how the intensity ratios between far apart group of lines are remarkably different between the experimental and computed spectrum; for example, the L-M lines appear much higher than the K-L ones in the experiment, whereas that relationship is inverted in the computed spectrum. The major factor contributing to this is the fact that the sensitivity of the instrument used to acquire the spectrum is not constant, but goes down as the energy increases, and the spectrum itself has not been corrected for this. If one focuses on individual groups of lines, such as the L-M, L-N and L-O ones, one sees that experimental and computed spectra exhibit similar patterns, as the lines are concentrated in a small enough interval of energies that the sensitivity of the instrument remains nearly constant. Another thing to consider, however, is that the intensities in the computed spectrum are based only on the probability of a transition to take place. In reality, the intensity will be controlled also by the
population of the upper state from which the decay takes place. The computed spectrum as it is produced now by mudirac does not account for differences in the probability of each state being populated, and assumes them to be all equally likely starting points for a transition. This is in practice not the case. In fact, the probability distribution in each of the states in the lower shells heavily depends on the cascade process and the starting angular momentum of the muon upon capture.\textsuperscript{[46,47]} The cascade can be computed given the transition rates, but one still needs to make assumptions about the initial angular momentum distribution. This is part of future plans for this project, but is currently not implemented in the software.

Figure 7 shows a comparison between experiment and computation for gold, up to 8000 keV. The gold spectrum was computed up to the P shell ($n = 6$). The comparison is split in different panels to highlight the details of the spectra at different scales; because the detector loses efficiency at high energy, the intensity has been re-scaled between panels to better show the lines. The range up to 1,000 keV uses data with a resolution of 0.5 keV; the 1000–8000 keV range uses data from a detector with a 2 keV resolution, which was the only one able to reach such high energies. The software allows us to identify various lines, from the K-L group at high energies (>5,000 keV) to the very low energy transitions in between states in the same shell (<150 keV). Interpretation of the spectrum, however, is in this case somewhat complicated by the fact that this vast range includes high-energy phenomena that are not only muon level transitions. Due to the high overlap between muon and nucleus, multiple nuclear reactions take place, resulting, for example, in the transmutation of gold to platinum by the reaction \( \mu^- + p^+ \rightarrow n + \nu \), with the excess energy ending up carried away by either the neutrino or the neutron, and the resulting nucleus being in an excited state that decays with emission of gamma rays. This kind of absorption and transmutation process is well known, and the figure shows the signature in particular of the reaction \(^{197}\text{Au} + \mu^- \rightarrow ^{196}\text{Pt} + n\), as several lines connected to the decay of excited states of \(^{196}\text{Pt}\) are identifiable (dashed lines in Figure 7).\textsuperscript{[48,49]} The 511 keV line corresponding to electron–positron annihilation can also be seen. In
addition, we can also see how the K1-L2 and K1-L3 lines, which have energies above 5 MeV, display single and double escape peaks at −511 and −1022 keV, a phenomenon related to the creation of electron–positron pairs and relative loss of energy in the measured photons. This is a well-known problem with germanium detectors in this energy range.[50] Finally, on the low energy end of the spectrum, the O2-O1 and O3-O1 muonic lines are likely hidden under the electronic K1-L2 and K1-L3 transitions of gold, at 67 and 68.8 keV, respectively,[51] excited by the cascade process of muons. The upper edge of the electronic X-ray spectrum for gold is at 80.7 keV, so we can be sure that no other lines are subject to this interference.[52]

Figures 8–10 show three more spectra and their interpretations, this time respectively carbon, copper and silver. These are similar to the previous examples, except for the fact that the carbon spectrum uses a Gaussian line broadening of only 0.5 keV. The carbon spectrum illustrates well how the spectra of light atoms are less
distinctive, as their signatures occupy a much smaller range of energies and only a few lines can be easily recognised.

Finally, we combine two of the previously seen spectra and consider the case of a two-element system; a 30–70 Au–Ag alloy. In this case, our objective is to distinguish peaks belonging to each element, allowing for some basic elemental analysis. The Au computed spectrum was the same used in the previous section; the Ag one was computed with the same parameters, and again up to the P shell \((n = 6)\). Figure 11 shows the results. Here we focus on the low energies, as this is where the spectra are more rich in features, and thus interpretation is usually more difficult. The same considerations as above are relevant for the electronic contributions to the spectrum; the upper edge of the spectrum for gold is 80.7 keV, while the one for silver is 25.5 keV,\(^{[53]}\) so we will limit ourselves to peaks higher than those energies, for which there is no risk of confusion.

Some peaks are highlighted with their respective assignments. The relative abundance of the two elements is reflected in the relative intensities of the peaks, with

**FIGURE 8** Experimental (top) and computed (bottom) X-ray spectrum for muonic carbon (graphite)

**FIGURE 9** Experimental (top) and computed (bottom) X-ray spectrum for muonic copper. The experimental spectrum shown is from a 94–6 Cu–Sn alloy, but only the copper component is analysed here, as it is by far the most visible.
the ones that can be unequivocally identified as originating in the gold, like the N–O group around 400 keV, being quite lower in intensity than the silver ones. One must also pay attention to potential sources of ambiguity: for example, around 216 keV, one peak can be assigned either as the O9-P11/O8-P10 doublet from gold or as the

Figure 10 Experimental (top) and computed (bottom) X-ray spectrum for muonic silver

Figure 11 Experimental (top) X-ray spectrum for muons in a 30–70 Au–Ag alloy. Below are the computed spectra for muonic gold (middle) and silver (bottom)
N7-P9/N5-P7 doublet from silver. It is hard to tell which of the two it is, and it could be a combination of both. Finally, another possible source of confusion must be considered in this low energy range: the lack of information about states above a certain energy. Computations were stopped at a given shell, which means that all transitions involving states above that are missing from our interpretation. As states get closer and closer in energy, going up in shells, more transition energies open up, leading to a nigh continuum of possible transitions in energy. This is further complicated by the fact that converging calculations for such higher states is also more difficult; in this example, the P10 and P11 states for Ag did not converge and the peaks they contribute to are missing from the spectrum. Going above this problem becomes only more severe, and affects our ability to properly interpret spectra in the low energy range. Improving these convergence properties is one of the future objectives for the development of the software.

6 | CONCLUSIONS

A software to solve the radial Dirac equation specifically designed for muonic atoms has been produced and released for public use under an open-source license. The software, called mudirac, is able to compute energies and transition rates for all the main X-ray spectral lines for muonic atoms across the periodic table, accounting for the most important effects such as the finite size of atomic nuclei and the Uehling correction. This provides a useful tool to help with the interpretation of muonic X-ray spectra for elemental analysis. The software has also been designed to easily accommodate future expansions such as the addition of more correction terms for its potential in order to achieve higher accuracy. In addition, future work will focus on using the software’s predictions for transition rates in order to help interpret line intensities based on a model of the muonic cascade, as well as improving its ability to compute states in higher shells.

ACKNOWLEDGEMENT

Thanks to Dominik Jochym Albert Bartok-Partáy, Beth Hampshire and Katsu Ishida for the useful discussions and contributions. The development of this software was funded by the Ada Lovelace Centre and was carried out by the Scientific Computing Department of STFC in collaboration with the ISIS Muon Group. The experimental data were acquired thanks to STFC providing the beamtime, and can be referenced as Dr Aidy Hillier et al. (2019), “How low can you go?”, STFC ISIS Neutron and Muon Source, https://doi.org/10.5286/ISIS.E.RB1820616-1. The raw data are stored within the ISIS Neutron and Muon Source data journal, and will become publicly available on March 11, 2022.

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