Mathematical formulation of the Dirac, Breit-Darwin equation for purely leptonic atoms

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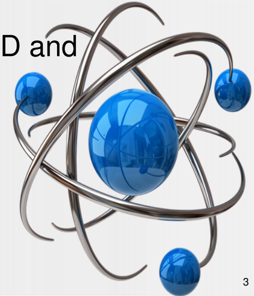
Outlook

1. Introduction
2. Exotic leptonic atoms (muonium, positronium, etc.)
3. Quantum mechanical description
   - Non-relativistic
   - Relativistic
4. Comparison of theoretical predictions with experimental data
5. Summary, conclusions and outlook

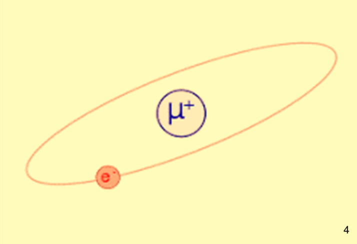
Introduction-Importance of Leptonic Atoms in BSM

- Conventional matter consist of leptons and quarks
- Some bosons are responsible for all the interactions
- Leptonic atoms are free of hadronic complex structure and effects $\longrightarrow$ ideal to investigate the QED and beyond the Standard Model physics
- High precision spectroscopy of Muonium is crucial in testing QED and in determining the m_e/m_μ ratio
- Importance in measuring the muon mass m_μ and fine structure constant α



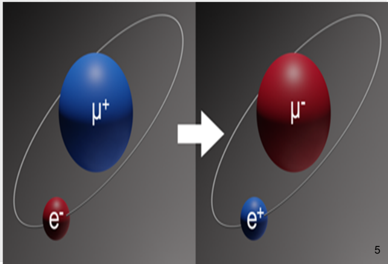
Muonium (Mu): Properties

- An exotic atom made up from an antimuon and an electron (μ^+ e^-) where the dominant interaction is electromagnetic
- It is formed when a positive muon captures an atomic electron after being slowed down in matter
- Due to the large muon's mass m_μ, it shares more similarities to hydrogen than positronium. It may be considered an exotic light isotope of hydrogen
- It is short-lived, with $\tau = 2, 2\ \mu s$, however it undergoes chemical reactions
- It is studied through "muon spin spectroscopy" (μSR)



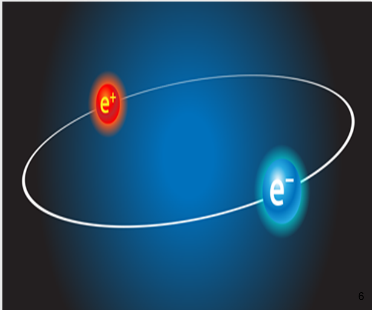
Muonium (Mu): Important Observables

- μSR is implemented in analysis of the structure of the compounds and chemical transformations
- Due to its leptonic nature, QED is able to predict its atomic energy levels with great precision
- Muonium is an ideal system for studying QED and for physics beyond the Standard Model (BSM)
- Conversion of Mu to $\overline{Mu}$ is effective in identifying fundamental interactions related to the lepton flavor and lepton number violation



Positronium (Ps): General Properties

- A leptonic atom consisting of a positron and an electron ($e^+ e^-$)
- It is formed as a positron is losing energy in matter and is captured by an electron
- This system is unstable as the two particles annihilate each other to produce gamma-rays
- Positronium participates in chemical bonding such as positronium hydride (PsH) and cyanide
- Ps exhibits great differences in size, polarizability and binding energy from hydrogen due to the similarities between e^+ and e^-

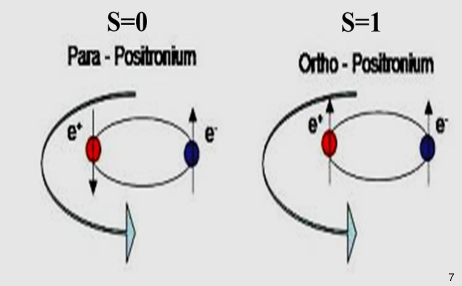


Positronium (Ps): QM-description

- The singlet state, S=0, (antiparallel spins) is known as para-positronium, p-Ps, with $\tau = 0,12$ *ns* $\longrightarrow$ decays into two photons

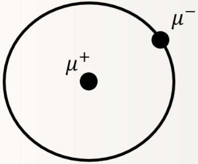
- The triplet state, S=1, (parallel spins) is called ortho-positronium, o-Ps, with a slightly higher energy than p-Ps and $\tau = 142$ *ns* $\longrightarrow$ decays into three photons

- Exhibits a hyperfine energy correction that is comparable to the respective fine structure one

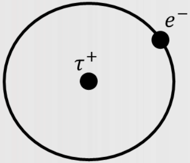


Other Leptonic Atoms

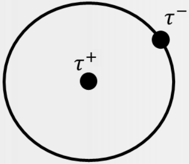
True Muonium



Tauonium

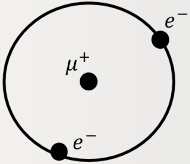


True Tauonium

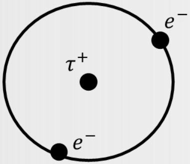


3-body lepton systems

Muonium ion



Tauonium ion



Quantum Mechanical Description of Purely Leptonic Atoms

- Non-relativistic
  - Schrödinger equation
  - Inclusion of relativistic corrections (fine structure terms)
- Relativistic
  - Two-body Dirac equation (relative coordinate system)
  - Inclusion of the Breit-Darwin terms
  - Inclusion of Lamb shift (self-energy, vacuum polarization, etc.)

Non-relativistic treatment

Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2\mu r^2}-\frac{e^2}{r}\right]u(r)=Eu(r)$$

Fine structure splitting

Breaking of the degeneracy of the energy levels due to the spin and relativistic corrections to the Schrödinger equation

I. Relativistic correction to the kinetic energy

II. Spin-orbit coupling

III. Darwin term

Derivation from the Non-relativistic limit of the Dirac equation

Analytical Solution of the Schrödinger Equation

Radial solution of the Schrödinger equation

$$R_{nl}(r) = \sqrt{\left(\frac{\bar{r}}{nr}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}} \left(\frac{\bar{r}}{n}\right)^l e^{-\bar{r}/2n} L_{n-l-1}^{2l+1}\left(\frac{\bar{r}}{n}\right),$$

$$\bar{r} = 2Zr/\alpha_0^*$$

Generalized Laguerre polynomials are the solution to:

$$x\frac{d^2}{dx^2}L_n^{(a)} + (a+1-x\frac{d}{dx}L_n^{(a)} + nL_n^{(a)} = 0, \quad a > -1$$

Examples of Laguerre polynomials

$$L_0^{(a)}(x) = 1, \qquad L_1^{(a)}(x) = -x + a + 1,$$

$$L_2^{(a)}(x) = \frac{x^2}{2} - (a+2)x + \frac{(a+1)(a+2)}{2}$$

Analytical Solutions for Leptonic Atoms

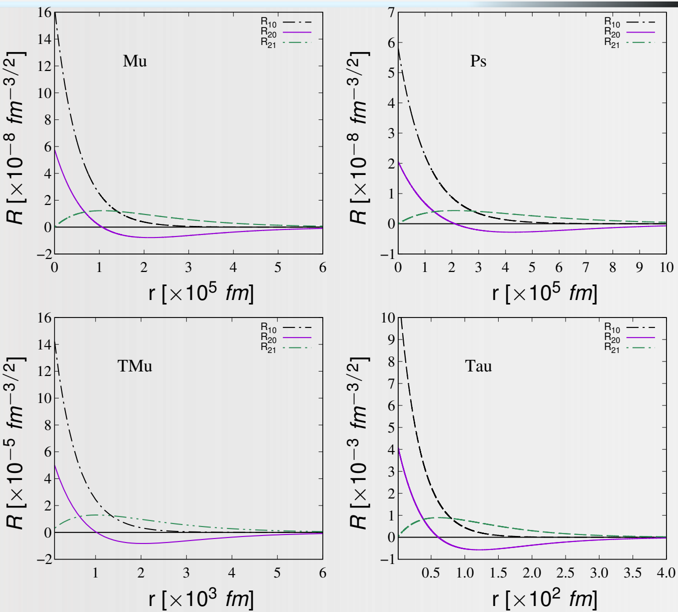
Analytical radial components of the first three orbitals

$$R_{10}(r) = 2\left(\frac{Z}{\alpha_0^*}\right)^{3/2} e^{-\bar{r}/2}$$

$$R_{20}(r) = \left(\frac{Z}{2\alpha_0^*}\right)^{3/2}\left(2-\frac{\bar{r}}{2}\right) e^{-\bar{r}/4}$$

$$R_{21}(r) = \left(\frac{Z}{2\alpha_0^*}\right)^{3/2}\frac{\bar{r}}{2\sqrt{3}} e^{-\bar{r}/4}$$

$$E_n = -\frac{\hbar^2}{2\mu\alpha_0^{*2} n^2}$$



Relativistic Treatment

- First attempt: Klein-Gordon equation → Inserts the energy and momentum operators from special relativity → Negative energy solutions-Missing spin
- Spin input: Weyl equation → Inclusion of the Pauli matrices → Only for massless spin-1/2 particles
- Solution: Dirac equation → Incorporation of special relativity in quantum mechanics → Describes all spin-1/2 particles

The Dirac Equation Formalism

$$[\gamma^\mu(i\partial_\mu - eA_\mu) - mc^2]\Psi = 0$$

$$(E - mc^2 - V(r))g\mathcal{Y}_{jlm} = \frac{1}{r}\frac{\boldsymbol{\sigma}\cdot\boldsymbol{r}}{r}\left[-ir\frac{\partial}{\partial r} + i\boldsymbol{\sigma}\cdot\boldsymbol{L}\right] if\mathcal{Y}_{jl'm}$$

$$(E + mc^2 - V(r))if\mathcal{Y}_{jl'm} = \frac{1}{r}\frac{\boldsymbol{\sigma}\cdot\boldsymbol{r}}{r}\left[-ir\frac{\partial}{\partial r} + i\boldsymbol{\sigma}\cdot\boldsymbol{L}\right] g\mathcal{Y}_{jlm}$$

The Dirac equation for a hydrogen-like atom

$$\boldsymbol{\sigma}\cdot\boldsymbol{L}\psi_A = (-k-1)\hbar\psi_A$$

$$\boldsymbol{\sigma}\cdot\boldsymbol{L}\psi_B = (k-1)\hbar\psi_B$$

$$k \rightarrow -k-1$$

$$E_{nj} = \frac{mc^2}{\sqrt{1 + \frac{(Z\alpha)^2}{\left(n-j-\frac{1}{2}+\sqrt{(j+1/2)^2-(Z\alpha)^2}\right)^2}}}$$

$$\frac{\partial}{\partial r}\begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} \frac{k-1}{r} & -\frac{E-V-\mu c^2}{\hbar c} \\ \frac{E-V+\mu c^2}{\hbar c} & -\frac{k+1}{r} \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix}$$

Eshetu Diriba Kena and Gashaw Bekele Adera (2021) J. Phys. Commun. 5 105018

The Dirac Equation Formalism

Dirac equation formalism

$$\frac{\partial}{\partial r}\begin{pmatrix} f(r) \\ g(r) \end{pmatrix} = \begin{pmatrix} \frac{k-1}{r} & -\frac{E-V-\mu c^2}{\hbar c} \\ \frac{E-V+\mu c^2}{\hbar c} & -\frac{k+1}{r} \end{pmatrix} \begin{pmatrix} f(r) \\ g(r) \end{pmatrix}, \quad k = \pm\left(j + \frac{1}{2}\right)$$

Hyperfine splitting (hfs)

Splitting of the energy levels due to interaction between the nuclear spin and electron movement

+

Lamb shift

Energy deviation between the first orbitals due to vacuum energy fluctuations

The Breit-Darwin Equation

$$\hat{H} = \hat{H}_i + \hat{H}_j + \hat{H}_{int}$$

$$\hat{H}_i = \frac{\hat{\boldsymbol{p}}_i^2}{2m_i} - \frac{\hat{\boldsymbol{p}}_i^4}{8c^2 m_i^3}$$ → Relativistic correction to the kinetic energy

$$\hat{V}_R = \frac{e^2}{2m_i m_j r c^2}\left[\hat{\boldsymbol{p}}_i \cdot \hat{\boldsymbol{p}}_j + \frac{(\boldsymbol{r}\cdot\hat{\boldsymbol{p}}_i)(\boldsymbol{r}\cdot\hat{\boldsymbol{p}}_j)}{r^2}\right]$$ → Retardation effects

$$\hat{V}_D^{(i)} = \frac{\pi e^2 \hbar^2}{2m_i^2 c^2}\delta(\boldsymbol{r})$$ → Zittebewegung-Darwin term

$$\hat{V}_{SO}^{(i)} = \frac{-q_i e \hbar^2}{4 m_i c^2 r^3}\left(\frac{\boldsymbol{r}\times\hat{\boldsymbol{p}}_i}{m_i} - \frac{\boldsymbol{r}\times\hat{\boldsymbol{p}}_j}{m_j}\right)\cdot\boldsymbol{\sigma}_i$$ → Spin-orbit interaction

$$\hat{V}_{hfs} = \frac{e^2\hbar^2}{4m_i m_j c^2}\left[\frac{3(\boldsymbol{\sigma}_i\cdot\boldsymbol{r})(\boldsymbol{\sigma}_j\cdot\boldsymbol{r}) - \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j}{r^3} + \frac{8\pi}{3}\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\delta(\boldsymbol{r})\right]$$ → Hyperfine structure hamiltonian

$$\hat{V}_{ext}^{(i)} = \frac{e\hbar}{m_i c}\left(\frac{\boldsymbol{H}\cdot\boldsymbol{\sigma}_i}{2} + \frac{q_i}{m_i c}\boldsymbol{A}\cdot\hat{\boldsymbol{p}}_i\right)$$ → Interaction with external magnetic field

Daza, F.G., Kelkar, N.G. and Nowakowski, M. (2012) J. Phys. G: Nucl. Part. Phys. 39 035103

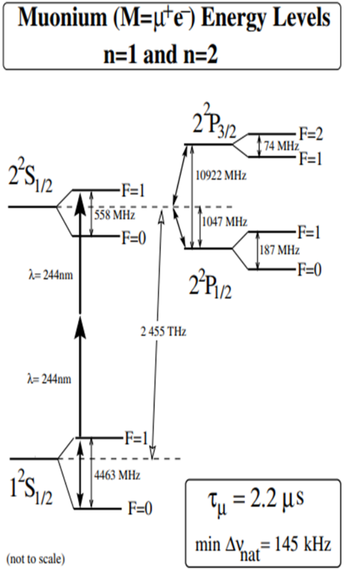
Mu spectroscopy

- Ground state hfs structure
- 1s-2s energy interval
- *Mu-M̄u* conversion
- Test of CPT and Lorentz invariance

Achievements

- Accuracy in values such as m_μ, μ_μ, α_μ, α
- Search for new unknown forces in nature
- Restrictions on parameters of speculative theories

Crivelli, P. (2018) Hyperfine Interact 239, 49

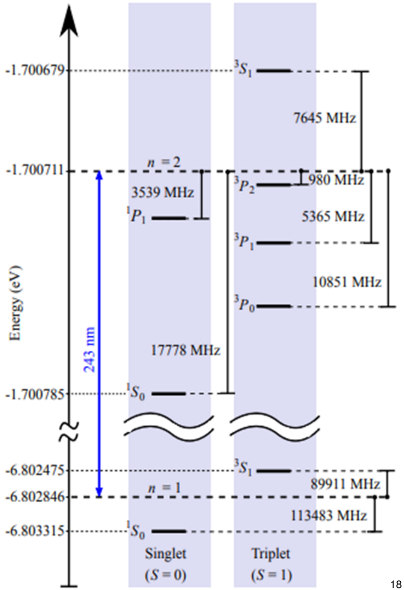


Ps spectroscopy

- Test of QED
- hfs on the ground state
- Maximal recoil effects
- Deexcitation of Rydberg Ps states

Achievements

- High accuracy in measuring the Rydberg constant
- Test fundamental symmetries
- Restrictions on the types of new forces, particles or fields invented to overcome the SM weaknesses



Cassidy, D.B. (2018)
Eur. Phys. J. D 72, 53

Experimental vs Theoretical Predictions

Theoretical predictions for Ps

Quantity	Prediction
$\Delta\nu(1S-2S)$	1 233 607 222.2(6) MHz
$\Delta\nu_{HFS}(1S)$	203 391.7(5) MHz
$\Delta\nu(2^3S_1-2^3P_0)$	18 498.25(9) MHz
$\Delta\nu(2^3S_1-2^3P_1)$	13 012.41(9) MHz
$\Delta\nu(2^3S_1-2^3P_2)$	8 625.70(9) MHz
$\Delta\nu(2^3S_1-2^1P_1)$	11 185.37(9) MHz
Γ(p−Ps)	7 989.32(2) μs^{-1}
Γ(o−Ps)	7.040 07(2) μs^{-1}

Mu	Theory (MHz)	Experiment (MHz)
1S-2S	2455528935,8(1,4)	2455528941,0(9,8)
Lamb shift	1047,284(2)	1042(22)
Ground state hfs	4463,30289(27)	4463,302765(53)
Ps	**Theory (MHz)**	**Experiment (MHz)**
1S-2S	1233607222,13(58)	1233607216,4(3,2)
Ground state hfs	203391,91(22)	203394,2(2,1)

Frugiuele, C., Perez-Ríos, J. and Peset, C. (2019) Phys. Rev. D 100, 015010

Important upcoming Mu experiments

- MuSEUM at J-PARC → the hfs structure
- Mu-MASS at PSI → 1S-2S transition frequency
- Muon g-2 at FNAL → anomalous magnetic moment

Conclusions

- Purely leptonic atoms offer promising research prospects in testing QED and BSM theories
- Mu and Ps are leading in the research interest due to their unique characteristics
- Accurate theoretical predictions require the solution of the Dirac equation, taking into account the Breit-Darwin terms and the Lamb shift
- Promising new experiments aim at shedding light on theoretical contradictions, especially concerning Mu
- Our goal is to make improved theoretical predictions for the leptonic atom bound states using advanced numerical codes

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

Thank you for your attention!

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OPRA

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$$f = \frac{1}{2} N e^{-\frac{\rho}{2}} \rho^{s-1} [M(s-\gamma,\ 2s+1,\ \rho) - L_- M(s-\gamma+1,\ 2s+1,\ \rho)$$
$$-\Lambda_+ \rho^{-2s} M(-s-\gamma,\ -2s+1,\ \rho) - \Lambda_- L_+ \rho^{-2s} M(-s-\gamma+1,\ -2s+1,\ \rho)]$$

$$g = \frac{1}{2} N \zeta e^{-\frac{\rho}{2}} \rho^{s-1} [M(s-\gamma,\ 2s+1,\ \rho) + L_- M(s-\gamma+1,\ 2s+1,\ \rho)$$
$$-\Lambda_+ \rho^{-2s} M(-s-\gamma,\ -2s+1,\ \rho)$$
$$+\Lambda_- L_+ \rho^{-2s} M(-s-\gamma+1,\ -2s+1,\ \rho)]$$

Where

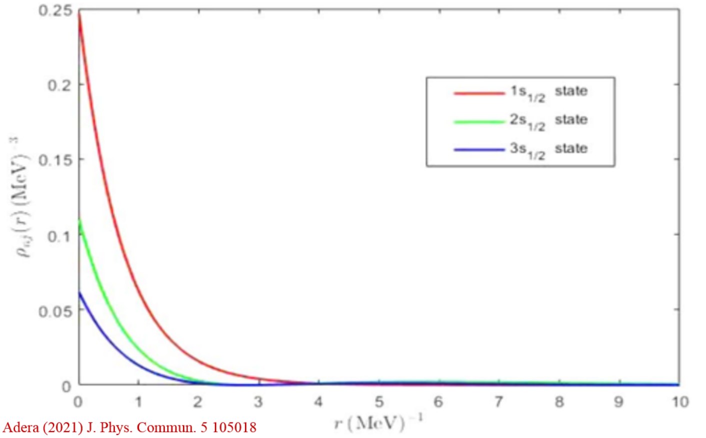
$$\Lambda_\pm = \frac{\Gamma(2s+1)}{\Gamma(-2s+1)} \frac{\Gamma\left(\frac{1}{2} - s - \beta_\pm\right)}{\Gamma\left(\frac{1}{2} + s - \beta_\pm\right)};\ L_\pm = \frac{s \pm \gamma}{\kappa - \gamma/E'};\ \ E' = \frac{E}{m}$$

And

$$\gamma = \frac{Z\alpha E'}{\sqrt{1 - E'^2}};\ \ \zeta = \sqrt{\frac{m-E}{m+E}};\ s = \sqrt{\kappa^2 - (Z\alpha)^2}$$

Probability density

$$\rho_{nj} = \begin{cases} \frac{1}{2j}\left(f^2 + \frac{j}{j+1}g^2\right), \, for \; j = l + \frac{1}{2} \\ \frac{1}{2j+2}\left(f^2 + \frac{j+1}{j}g^2\right), \, for \; j = l - \frac{1}{2} \end{cases}$$



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