Max-Planck-Institut für Kernphysik Heidelberg

MAX PLANCK GESELLSCHAFT

An updated computational tool for solving the radial wave equations

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Content

- The radial wave equations
- Currently available software
- What we do
- Some computational details
- Conclusion

The radial wave equations

Schrödinger case

electron (or positron) stationary states in non-relativistic quantum mechanics

spherical harmonics

$$\Psi_{Elm}(\mathbf{r}) = \frac{1}{r} P_{El}(r) Y_{lm}(\hat{\mathbf{r}})$$

distance from center

solve radial Schrödinger equation for P:

$$-\frac{\hbar^2}{2m_e}\frac{d^2 P_{El}}{dr^2} + \left[\frac{\hbar^2}{2m_e}\frac{l(l+1)}{r^2} + V(r)\right] P_{El} = E P_{El}$$

central potential

Dirac case

stationary states of relativistic elementary particles with spin ½

$$\Psi_{W\kappa m}(\mathbf{r}) = \frac{1}{r}\begin{pmatrix} P_{W\kappa}(r)\Omega_{\kappa,m}(\hat{\mathbf{r}}) \\ iQ_{W\kappa}(r)\Omega_{-\kappa,m}(\hat{\mathbf{r}}) \end{pmatrix}$$

(l-j)(2j+1)

spherical spinors

solve radial Dirac equations for P & Q:

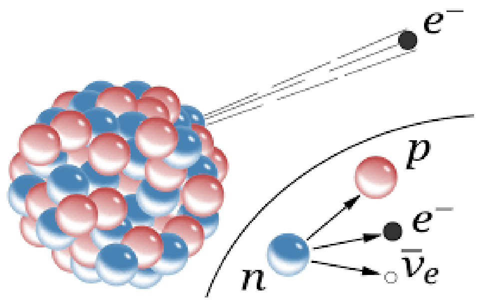
$$\frac{dP_{W\kappa}}{dr} = -\frac{\kappa}{r} P_{W\kappa} + \frac{W + m_e c^2 - V(r)}{c\hbar} Q_{W\kappa}$$

$$\frac{dQ_{W\kappa}}{dr} = \frac{-W + m_e c^2 + V(r)}{c\hbar} Q_{W\kappa} + \frac{\kappa}{r} Q_{W\kappa}$$

The radial wave equations – what for?

Needed for atomic and nuclear physics

e.g. beta decay (phase space)



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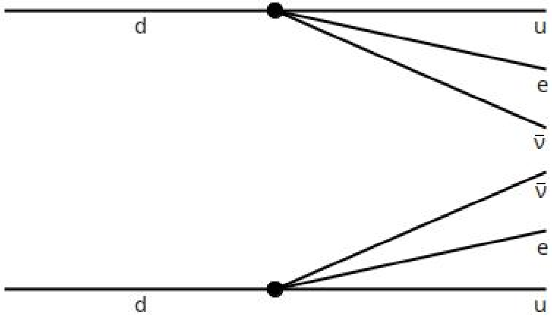

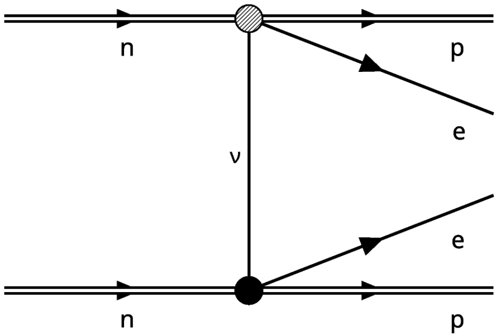

Currently available software

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C                                                                      C
C             RRRRR     AA     DDDDD    IIII     AA     L              C
C             R    R   A  A    D    D    II     A  A    L              C
C             R    R  A    A   D    D    II    A    A   L              C
C             RRRRR   AAAAAA   D    D    II    AAAAAA   L              C
C             R  R    A    A   D    D    II    A    A   L              C
C             R   R   A    A   DDDDB    IIII   A    A   LLLLLL         C
C                                                                      C
C                                                     (version 2018).  C
C                                                                      C
C  Numerical solution of the Schrodinger (S) and Dirac (D) radial      C
C  wave equations. Cubic spline interpolation + power series method.   C
C                                                                      C
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C
C  References:
C  [1] F. Salvat and R. Mayol,
C      'Accurate numerical solution of Schrodinger and Dirac wave
C      equations for central fields'.
C      Comput. Phys. Commun. 62 (1991) 65-79.
C  [2] F. Salvat, J. M. Fernandez-Varea and W. Williamson, Jr.,
C      'Accurate numerical solution of the radial Schrodinger and Dirac
C      wave equations'.
C      Comput. Phys. Commun. 90 (1995) 151-158.
C  [3] F. Salvat and J.M. Fernandez-Varea,
C      'RADIAL: a FORTRAN subroutine package for the solution of the
C      radial Schrodinger and Dirac wave equations'.
C      Internal report, University of Barcelona, 2018.
C      This document describes the RADIAL subroutine package and its
C      operation. The PDF file is included in the distribution package.
```

RADIAL: a Fortran subroutine package for the solution of the radial Schrödinger and Dirac wave equations

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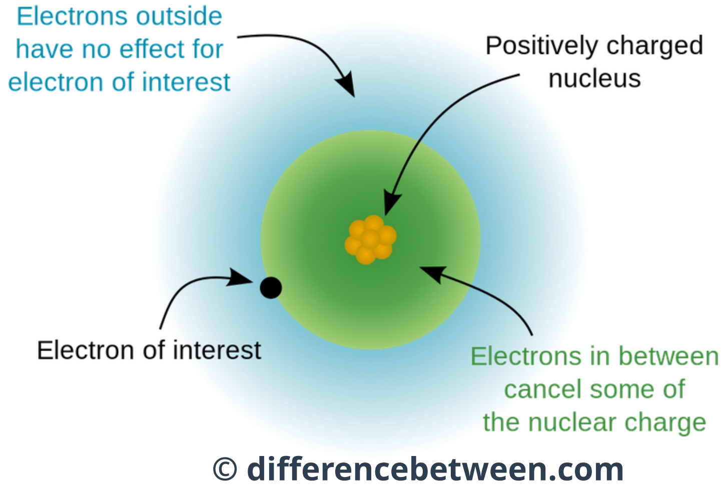
What we do

- **Easy to use Python package**
- **For both Schrödinger and Dirac radial wave equations & free and bound states**
- **Include electron screening**



Thomas-Fermi approximation

$$V(r) = \phi(r)V_0(r) \qquad \frac{d^2\phi}{dx^2} = \frac{\phi^{3/2}}{\sqrt{x}}$$

Some computational details

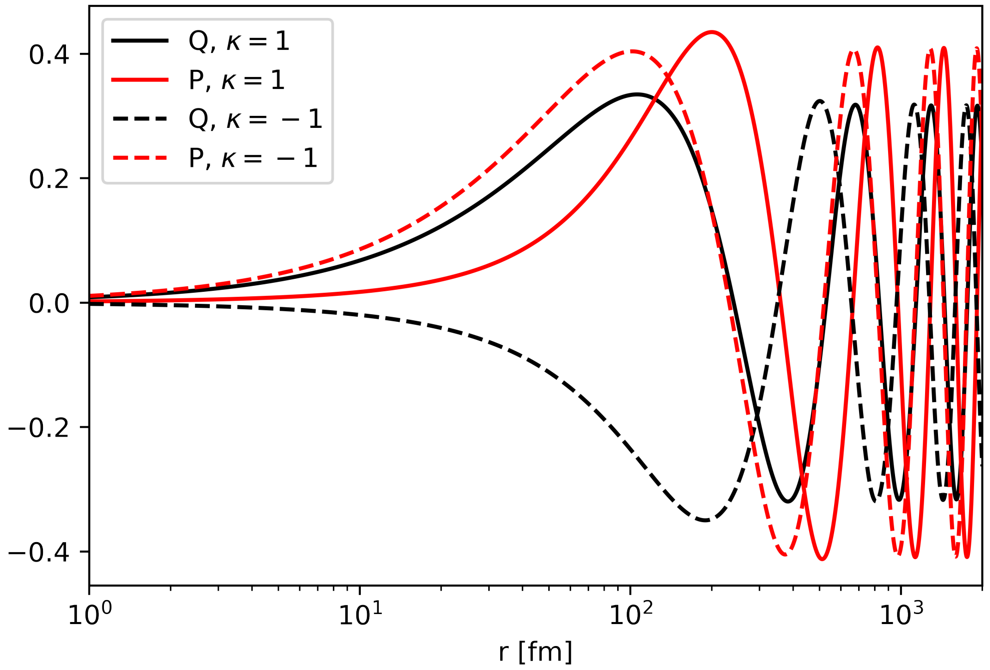
- For both Schrödinger and Dirac equation a numerical solution is extended outwards on a grid in r
- Power series ansatz for each interval; get coefficients from the wave equation
- If solution starts at r=0, some modifications are needed

Some computational details - normalization

- **Difference between bound and free states**
  - Bound states: Integrate over all intervals and use the sum of these contributions to normalize to one
  - Free states:
    - Find outer solution analytically assuming a Coulomb potential
    - Match inner solution with outer solution at a critical radius r_{crit}

For details please come to my poster/talk to me during breaks!

Some computational details – outer solution



Radial Dirac wave functions for ^{136}Xe with an electron energy of 2 MeV assuming a Coulomb potential.

Conclusions

- **Solution of radial wave equations essential for atomic and nuclear physics**
- **We are working on an easy to use Python package to solve the radial wave equations**
- **For Schrödinger & Dirac and free & bound states**

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Thank you for your attention!