DIRAC: Computer-Algebra Tool for Studying the Structure and Dynamics Highly-Charge, Heavy Ions

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Introduction: “hydrogen atom model” in modern physics

DIRAC computer algebra tool
  - A brief historical overview
  - General structure of the program
  - Interactive work with DIRAC: “Textbook examples”
  - Making physics with DIRAC: Advanced studies

Conclusion: Present and future of DIRAC package
Today, the ‘hydrogen atom model’ is known to play its role not only in teaching the basic elements of quantum mechanics but also for building up effective theories in atomic and molecular physics, quantum optics and plasma physics.
Analytical as well as numerical solutions of the hydrogen-like ions are frequently required both, for analyzing experimental data and for carrying out quite advanced studies.

Despite of all the knowledge about the hydrogen-like ions, the mathematics of this model is not always easy to deal with.

Rather usual it is not easy to get access to the necessary information.

Fast and reliable access to properties and solutions of hydrogen-like ions is highly required in nowadays studies!
A large number of computer code have been developed over the last decades to deal with the “hydrogen atom model”


and many others programs which have been certainly found useful for understanding the properties and behavior of one-electron atoms and ions.

These programs are often designed to solve some particular tasks and can not be extended so easily to other problems.

Fast and reliable access (based on computer algebra system) to properties and solutions of hydrogen-like ions is highly required in nowadays studies!
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1999 - 2000: Idea of DIRAC as a set of procedures for analytical and numerical evaluation of wavefunctions, matrix elements, cross sections, etc.

2005: First realization of DIRAC program as a set of MAPLE procedures.

2006 - 2008: Application of DIRAC to various research projects, getting “feedback” from users.

2009: New DIRAC based on MATHEMATICA language.
Our philosophy: DIRAC package is organized in hierarchical order where each command can be either used for interactive work or simply as a language element for building up commands at some higher level of hierarchy.

Roughly speaking: DIRAC is a set of MATHEMATICA procedures. (Note additional prefix Dirac in order to distinguish from “built-in” procedures).

From more than 60 procedures (present status) only about 15 procedures of top level to be known by the user.
**Concept of settings (which are saved in global variables)**

- System of units
- Nuclear charge $Z$
- Relativistic/nonrelativistic

**User may define a proper framework by making use of `DiracSettings[... ]` procedure.**

**Charge: $Z > 0$**

```
In[4]:= DiracSettings[charge, 92]
Out[4]= The charge is set to 92
```

**Framework: relativistic or nonrelativistic**

```
In[5]:= DiracSettings[units, natural]
Out[5]= The units is set to natural
```

```
In[6]:= DiracSettings[framework, relativistic]
Out[6]= The framework is set to relativistic
```
You might have recognized already: concept of keywords: one may control input/output of particular procedure (element of DIRAC) by proper choice of keywords!

- User may define a proper framework by making use of DiracSettings[... ] procedure.

**Atomic**

\[ e = m_e = \hbar = 1 \]

**Natural**

\[ c = m_e = \hbar = 1 \]

**Units**

**SI**

\[ \eta = \frac{e}{m} = \frac{\hbar}{c} = 1 \]

**Framework:** relativistic or nonrelativistic

**Charge:** \( Z > 0 \)

\[ \text{In}[4] := \text{DiracSettings}[\text{charge}, 92] \]

\[ \text{Out}[4] = \text{The charge is set to 92} \]

\[ \text{In}[5] := \text{DiracSettings}[\text{units}, \text{natural}] \]

\[ \text{Out}[5] = \text{The units is set to natural} \]

\[ \text{In}[6] := \text{DiracSettings}[\text{framework}, \text{relativistic}] \]

\[ \text{Out}[6] = \text{The framework is set to relativistic} \]
We make use of the MATHEMATICA functionality we support interactive help support!
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Example: Fine-structure of H-like ions

Welcome to the Dirac Package.

Version 9.06.2

The default values are:

DiracSaveFramework = nonrelativistic
DiracSaveCharge = Z
DiracSaveUnits = atomic

For help, see DiracDocumentation

\[ n_2 = \text{DiracSettings}[\text{framework, relativistic}] \]
\[ \text{Out}[2]= \text{The framework is set to relativistic} \]

\[ n_4 = \Delta E = \text{DiracEnergy}[2, -2] - \text{DiracEnergy}[2, 1] \]

\[ \Delta E = \frac{\alpha^2}{\sqrt{1 + \frac{2^2 \alpha^2}{4 - 2^2 \alpha^2}}} - \frac{1}{\sqrt{1 + \frac{2^2 \alpha^2}{1 + 4 - 2^2 \alpha^2}}} \]

\[ \text{Out}[4]= \frac{\alpha^2}{2} \frac{Z^4}{32} + O[Z]^5 \]

Fine structure splitting between \(2p_{3/2} (n=2, \kappa=-2)\) and \(2p_{1/2} (n=2, \kappa=1)\) states of hydrogen-like ions.
Example: Relativistic contraction of s-orbitals

\begin{verbatim}
In[26]:= DiracSettings[charge, 92]
Out[26]= The charge is set to 92

In[28]:= DiracSettings[framework, relativistic]
Out[28]= The framework is set to relativistic

In[31]:= PR = DiracRadialComponent[large, 4, -1, r];

In[32]:= DiracSettings[framework, nonrelativistic]
Out[32]= The framework is set to nonrelativistic

In[35]:= PNR = DiracRadialOrbital[4, 0, r]
Out[35]= \(46 \sqrt{23} \ e^{-23 \ r} \ r \left(1 - 0.69 \ r + 1.058 \ r^2 - \frac{12.167 \ r^3}{3}\right)\)

In[37]:= Plot[{PR, PNR}, {r, 0, 1}, PlotRange -> All]
\end{verbatim}
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Apart from the “textbook” example DIRAC have been already applied to many case studies on the structure and dynamics of heavy, few-electron ions.

For example, making use of DIRAC toolbox, calculations have been performed for:

- Radiative electron capture (REC)
- by heavy ions

**DiracMatrixElement[...]**
**DiracCrossSection[...]**

- REC cross sections
- angular distributions
- polarization

Apart from the “textbook” example, DIRAC has been already applied to many case studies on the structure and dynamics of heavy, few-electron ions.

For example, making use of the DIRAC toolbox, calculations have been performed for:

- Two-photon decay of H-like ions
  - DiracGreensFunction[…]
  - DiracCrossSection[…]
  - total rates
  - angular correlations
  - entanglement

Apart from the “textbook” example DIRAC have been already applied to many case studies on the structure and dynamics of heavy, few-electron ions.

For example, making use of DIRAC toolbox, calculations have been performed for:

- Coulomb excitation in relativistic ion-atom collisions
- DiracMatrixElement[…]
- DiracCrossSection[…]
- total cross sections
- alignment

A. Surzhykov et al., PRA 77 (2008) 042722
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Dirac package: Present and future

- September 2009: “DIRAC I” will be released (web, CPC)

- Spring 2010: “DIRAC II” will be released

- Autumn 2010: “DIRAC III” will be released

**Wavefunctions and integrals**
- wavefunctions (different representations)
- Greens functions
- energies
- radial integrals involving wavefunctions

**Interaction with radiation**
- photoionization and recombination
- radiative decay and absorption
- two-photon transitions

**Many-electron models?**
- Atomic collisions?
If you are interested in DIRAC package, please, contact us:

- E-mail: surz@physi.uni-heidelberg.de
- Web: http://www.physi.uni-heidelberg.de/Forschung/apix/TAP/index.php (from September)

Code of the program in CPC library: ADUQ

Thank you very much for your attention!