Evaluation of the Fundamental Physical Constants in *Mathematica*

Andrey S. Siver

Institute of High Energy Physics, Protvino, Russia

Abstract. We present PAREVAL package consisting of a number of *Mathematica* modules used to re-evaluate basic CODATA:1998 recommended fundamental physical constants (FPC). Package can be found at http://sirius.ihep.su/∼siver. Values of the basic FPC-1998 with the positive defined correlation matrix and a number of functions for the FPC usage can be found therein. Among other PAREVAL functions there are functions for energy levels of hydrogen and deuterium, electron and muon magnetic moment anomaly and muonium ground-state hyperfine splitting.

1 Introduction

Hopes for the discovery of new physics at present time are frequently connected with high-precision experiments combined with corresponding high-precision calculations. These calculations usually involve values of the FPC and should also use their uncertainties and correlation matrix. But none of the available resources provides the last one (correlation coefficients presented on the official site [3] are incorrect because they are rounded to three decimal figures).

Design of PAREVAL package has been mostly motivated by two facts:

– Methodological doubt about validity of CODATA recommended FPC-1998 [1]. This doubt arises due to the non-positive semi definiteness of the correlation matrix of the input experimental data presented in [1]. More information can be found in [4];
– Absence of powerful IT resources for scientific activities in FPC studies. Critical notes about several resources can be found in [4]

Our FPC-1998 re-evaluation has been generally based on review [1]. We have checked the values of the basic FPC and got their correlation matrix. The rest (derived) FPC can be expressed as a functions of the basic ones and thus be calculated.

2 Package Structure

PAREVAL consists of a number of *Mathematica* [2] modules which can be ranged as followings:

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1. Modules for FPC usage. Contains data and functions for the FPC usage in high-precision calculations;
2. Modules with physical formulae collection. Contains functions designed to calculate energy levels of hydrogen and deuterium, electron and muon magnetic moment anomaly, muonium ground-state hyperfine splitting and some other functions;
3. Modules for experimental data processing. Contains functions transforming experimental data between input and internal forms;
4. Module for parameters evaluation. Contains *Mathematica* functions for evaluation of parameters based on least-squares method;
5. Modules for results presentation. Contains functions used to present results of parameters evaluation in LaTeX system.

The package has general public license (GPL) [5] and can be found at http://sirius.ihep.su/∼siver. Values of the basic FPC-1998 with the positive defined correlation matrix, a number of useful functions for the FPC usage, *Mathematica* notebook in which calculations have been carried out can be found therein.

Most important modules are in a nutshell described below.

2.1 Modules for FPC Usage

The first module contains several *Mathematica* variables which can be used in calculations. The second one contains a function for the calculation of the FPC uncertainties propagation with FPC covariance matrix.

Module	Function	Input	Output	Example	Description of the symbols
fpc-usage-1	prop	f(z)	u[f(z)]	Fig.1	Calculates propagation of the uncertainties of the FPC for f(z) according to the law: $u[f(z_1,...,z_n)] = \sqrt{\sum_{i,j=1}^{N} \frac{\partial f}{\partial z_i} cov[z_i, z_j] \frac{\partial f}{\partial z_j}}$
fpc-usage-1	info	const	name, unit, symbTeX	Fig.1	name — ‘const’s name; unit — ‘const’s unit; symbTeX — ‘const’s TeX symbol

2.2 Modules with Physical Formulae Collection

These modules contain some realization of several physical functions used in FPC-1998 evaluations.

Function name	Mathem. symbol	Description
E1tot	$E_X(n, \mathrm{L}, j)$	Energy levels of hydrogen and deuterium[1]
a_e	a_e	Electron magnetic moment anomaly [1]
a_μ	a_μ	Muon magnetic moment anomaly[1]
$\Delta\nu_{Mu}$	$\Delta\nu_{Mu}$	Muonium ground-state hyperfine splitting [1]
ν	ν	Function conjugated to muonium ground-state hyperfine splitting([1], p.387)

Module	Func.	Input	Example	Description of the symbols
cod-15-3	E1tot	X, n, L, j	Fig. 2	X=(1 or 2), X=1 for hydrogen and X=2 for deuterium; n — principal quantum number; L — nonrelativistic orbital angular momentum; j — angular momentum quantum number;
formulae-2	a_e	alpha, dae		alpha — fine structure constant; dae — value of theoretical uncertainty for a_e (see [1], p.476).
formulae-2	a_μ	alpha, damu		alpha — fine structure constant; damu - value of theoretical uncertainty for a_μ (see [1], p.479).
formulae-2	$\Delta\nu_{Mu}$	mE, mM, aMU, alpha, R	Fig.3	alpha — fine structure constant; mE — electron mass; mM — muon mass; R — Rydberg constant. aMU — Muon magnetic moment anomaly

```
In[7]:= dir1 = "d:\\siver\\4mathematica\\par-0.9.2\\";

In[8]:= << (dir1 <> "reFPC-1998-2.m"); << (dir1 <> "fpc-usage-1.m");

In[9]:= info[R]

Out[9]= {Rydberg constant, m^-1, R_{\infty}}

In[10]:= info[hPl]

Out[10]= {Planck constant, J s, h}

In[11]:= info[alpha]

Out[11]= {fine-structure constant, 1, \alpha}

In[12]:= m_e = R / alpha ^2 / c * 2 * hPl /. c -> 299792458;
         val = m_e /. subsFPC (* === get value === *)

Out[13]= 9.10938187149259 × 10^-31

In[14]:= unc = prop[m_e] (* === get uncertainty === *)

Out[14]= 7.20642221827284 × 10^-38

In[15]:= unc / val (* === get relative uncertainty === *)

Out[15]= 7.91098926352514 × 10^-8
```

Fig. 1. Example of the usage of modules for calculations with the FPC

```
In[12]:= Collect[
          Simplify[
           Expand[
            (E1tot[HH, 2, 0, 1/2] - E1tot[HH, 1, 0, 1/2]) /.
                {Z → 1, mN → mp, m1 → mp, RR[1] → RP} /. me → 9.109381874910758 * 10 ^ (-31) /.
              mp → 1.672621582915101 * 10 ^ (-27) /. mμ -> 1.883531087707727 * 10 ^ (-28) /.
            c → 299792458], α > 0 && α < 1/2], α]
```

$$
\text{Out[12]=}\ -2.22578\times 10^{-17}\,\alpha^{2} - \frac{1.40384\times 10^{-55}\,\mathrm{RP}^{2}\,\alpha^{4}}{h^{2}} + \frac{1}{8}\left(8.90312\times 10^{-17} + 497.\,h - 6.55057\times 10^{-13}\sqrt{1-\alpha^{2}} + 4.63132\times 10^{-13}\sqrt{1+\sqrt{1-\alpha^{2}}}\right) +
$$

$$
\frac{1}{8}\,\alpha^{5}\left(5.76497\times 10^{-13} + \frac{3.27423\times 10^{-75}\,\mathrm{RP}^{3}}{h^{3}} + 4.85732\times 10^{-13}\,\mathrm{Log}[\alpha]\right) +
$$

$$
\frac{1}{8}\,\alpha^{8}\,(2.50237\times 10^{-14} - 3.1776\times 10^{-16}\,\mathrm{Log}[\alpha] + 5.83615\times 10^{-13}\,\mathrm{Log}[\alpha]^{2}) +
$$

$$
\frac{1}{8}\,\alpha^{7}\,(7.04894\times 10^{-12} + 1.89846\times 10^{-12}\,\mathrm{Log}[\alpha] + 7.28499\times 10^{-13}\,\mathrm{Log}[\alpha]^{2}) +
$$

$$
\frac{1}{8}\,\alpha^{6}\left(-1.78255\times 10^{-12} + \frac{2.12019\times 10^{-54}\,\mathrm{RP}^{2}}{h^{2}} + \frac{1.12307\times 10^{-54}\,\mathrm{RP}^{2}\,\mathrm{Log}\left[\frac{1.71496\times 10^{-21}\,\mathrm{RP}\,\alpha}{h}\right]}{h^{2}}\right)
$$

Fig. 2. Lamb shift. Example of the usage of the 'E1tot' function. Unfortunately, it's impossible to show the expression for classical Lamb shift in a reasonable form obtained as *Mathematica* output. So we make extra substitutions for $\mathrm{m_e}$, $\mathrm{m_p}$, m_μ and c using the values of FPC-1998.

3 Further Work. Discussion

A long time ago it was realized that evaluation of the FPC gave two important results: (i) values of the FPC and (ii) test for modern theories on agreement with each other and with experiments [1].

The first task can be solved with the help of PAREVAL package. But in order to solve the second one a system for monitoring the values of FPC should be created. This system should include:

- Collection of methods for adjustment of parameters of the theories;
- A database of all measured experimental data which can be used in parameters evaluation;
- A database of all self-consistent modern theoretical formulae, relevant to the experimental database. Besides, the database of the formulae should be connected to calculation media;
- Collection of methods that could test statistical hypotheses and seek possible systematical errors or uncertainties of calculation methods and programming "bugs";
- Subsystem for the presentation of results;

```
In[38]:= temp = Simplify[Expand[ΔνMu[me, mμ, aμ, α, R] /. subsX /. dMu → 0],
           α > 0 && α < 1]
```

$$
\begin{aligned}
\text{Out[38]=}\ & 175-\frac{8\,c\,R\,\alpha^4\,(13+36\,\mathrm{Log}[2])\,m_e^2}{9\,(m_e+m_\mu)^3}+\frac{1}{135\,(m_e+m_\mu)^5}\\
&\Bigg(4\,c\,R\,\alpha^3\,m_e^2\,m_\mu\Bigg(650\,\alpha\,m_\mu^2-1440\,\alpha\,\mathrm{Log}[2]\,m_\mu^2-360\,\alpha\,\mathrm{Log}[\alpha]\,m_\mu^2+\\
&\frac{540\,\mathrm{Log}\left[\frac{m_\mu}{m_e}\right]m_\mu^2\,(m_e+m_\mu)}{\pi\,(m_e-m_\mu)}+30\,\alpha\,(m_e+m_\mu)^2+\frac{700\,\alpha\,(m_e+m_\mu)^2}{\pi^2}+\\
&\frac{7758\,\alpha^2\,(m_e+m_\mu)^2}{\pi^3}-\frac{10260\,\alpha^2\,(m_e+m_\mu)^2}{\pi}+\frac{840\,\alpha^2\,\mathrm{Log}[\alpha]^2\,(m_e+m_\mu)^2}{\pi}+\\
&\frac{195\,\alpha\,\mathrm{Log}\left[\frac{m_\mu}{m_e}\right](m_e+m_\mu)^2}{\pi^2}+\frac{540\,\alpha^2\,\mathrm{Log}[\alpha]\,\mathrm{Log}\left[\frac{m_\mu}{m_e}\right](m_e+m_\mu)^2}{\pi}-\\
&\frac{360\,\alpha\,\mathrm{Log}\left[\frac{m_\mu}{m_e}\right]^2(m_e+m_\mu)^2}{\pi^2}+\frac{240\,\alpha^2\,\mathrm{Log}\left[\frac{m_\mu}{m_e}\right]^2(m_e+m_\mu)^2}{\pi^3}-\\
&\frac{240\,\alpha^2\,\mathrm{Log}\left[\frac{m_\mu}{m_e}\right]^3(m_e+m_\mu)^2}{\pi^3}+\frac{1890\,\alpha\,(m_e+m_\mu)^2\,\mathrm{Zeta}[3]}{\pi^2}\Bigg)\Bigg)-\\
&\frac{1}{607500\,\pi^3\,(m_e+m_\mu)^3}\Big(c\,R\,\alpha^2\,(1+a_\mu)\,m_e\,m_\mu^2\\
&\Big(358500\,\pi^4\,\alpha^3-135000\,\pi^3\,(24+51\,\alpha^4+2\,\alpha^2\,(-11+\mathrm{Log}[64]))+\\
&4500\,\pi^2\,\alpha^3\,(1124-3840\,\mathrm{Log}[2]+15\,\pi\,\alpha\,(-547+240\,\mathrm{Log}[2]))\,\mathrm{Log}[\alpha]+\\
&4320000\,\pi\,\alpha^3\,(2\,\pi+\alpha)\,\mathrm{Log}[\alpha]^2+8\,\pi^2\,\alpha\,(-202500+4860000\,\alpha^3+\alpha^2\\
&(-15709037+13410000\,\mathrm{Log}[2]+562500\,\mathrm{Log}[2]^2-466875\,\mathrm{Zeta}[3]))+\\
&22500\,\pi\,\alpha^2\,(-197+12384\,\alpha^2-108\,\mathrm{Zeta}[3])-625\,\alpha^3\,\Big(28259+7200\\
&\mathrm{Log}[2]^4+172800\,\mathrm{PolyLog}\left[4,\frac{1}{2}\right]+40032\,\mathrm{Zeta}[3]-46440\,\mathrm{Zeta}[5]\Big)\Big)\Big)
\end{aligned}
$$

Fig. 3. Example of the usage of the '$\Delta\nu_{Mu}$' function - muonium ground-state hyperfine splitting

– Subsystem for automatical or semi-automatical search for scientific information (old, modern and which just have appeared), which can be helpful to researcher.

As far as we know, none of such systems actually exists. PAREVAL package can be considered as a prototype of such system.

At last we would like to note that our working experience in *Mathematica* tells us that this computer algebra system is powerful enough to realize a system for monitoring values of fundamental physical constants.

References

1. P. J. Mohr and B. N. Taylor, "CODATA recommended values of the fundamental physical constants: 1998", Rev. Mod. Phys. **72** (2000) 351.
2. *Mathematica*, http://www.wolfram.com
3. Fundamental Physical Constants from NIST, http://physics.nist.gov/cuu/Constants/
4. Siver A.S., Ezhela V.V., "On the CODATA recommended values of the fundamental physical constants: V3.2(1998)&V4.0(2002)", IHEP Preprint 2003-34, Protvino, 2003; arXiv:physics/0401064
5. For General Public License (GPL) note see http://www.gnu.org