Effects of variation of fundamental constants and violation of symmetries P, T, CPT in nuclei and atoms

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Astrophysical evidences for space-time variation of fundamental constants and proposals of laboratory tests

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Cosmology J.Barrow

Quasar data J.Webb, M.Murphy, J.King, S.Curran, M.Drinkwater, P.Tsanavaris, C.Churchill, J.Prochazka, A.Wolfe, S.Muller, C.Henkel, F.Combes, T.Wiklind, R.Carswell, M.Bainbridge


Molecular calculations: A. Borschevsky, M. Ilias, K.Beloy, P. Schwerdtfeger
Since variation of **dimensional** constants cannot be distinguished from variation of **units**, it only makes sense to consider variation of **dimensionless** constants.

- **Fine structure constant** \( \alpha = \frac{e^2}{2\varepsilon_0 hc} = 1/137.036 \)
- **Electron or quark mass/QCD strong interaction scale**, \( m_{e,q}/\Lambda_{QCD} \)
  \[ \alpha_{strong}(r) = \text{const}/\ln(r \Lambda_{QCD}/ch) \]

**Electron-to-proton mass ratio** = const \( m_e/\Lambda_{QCD} \)
Search for variation of fundamental constants

• Big Bang Nucleosynthesis
• Quasar Absorption Spectra
• Oklo natural nuclear reactor
• Atomic clocks
• Enhanced effects in atoms, molecules and nuclei
• Dependence on gravity

1 Based on atomic and molecular calculations
Evidence for spatial variation of the fine structure constant $\alpha$

Quasar spectra

Webb, King, Murphy, Flambaum, Carswell, Bainbridge, PRL2011, MNRAS2012

\[ \alpha(x) = \alpha(0) + \alpha'(0) x + \ldots \]

\[ x = r \cos(\phi), \quad r = ct - \text{distance (t - light travel time, c - speed of light)} \]

Reconciles all measurements of the variation
“Fine tuning” of fundamental constants is needed for life to exist. If fundamental constants would be even slightly different, life could not appear!

Variation of coupling constants in space provide natural explanation of the “fine tuning”: we appeared in area of the Universe where values of fundamental constants are suitable for our existence.

There are theories which suggest variation of the fundamental constants in expanding Universe.
Quasars: physics laboratories in the early universe
Use atomic calculations to find $\omega(\alpha)$.

For $\alpha$ close to $\alpha_0$, $\omega = \omega_0 + q(\alpha^2/\alpha_0^2 - 1)$

$q$ is found by varying $\alpha$ in computer codes:

$$q = d\omega/dx = [\omega(0.1) - \omega(-0.1)]/0.2, \quad x = \alpha^2/\alpha_0^2 - 1$$

$\alpha = e^2/2 \varepsilon_0 hc \approx 0$ corresponds to non-relativistic limit (infinite $c$). Dependence on $\alpha$ is due to relativistic corrections.
### Methods of Atomic Calculations

<table>
<thead>
<tr>
<th>$N_{ve}$</th>
<th>Relativistic Hartree-Fock $+$</th>
<th>Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>All-orders sum of dominating diagrams</td>
<td>0.1-1%</td>
</tr>
<tr>
<td>2-6</td>
<td>Configuration Interaction $+$ Many-Body Perturbation Theory</td>
<td>1-10%</td>
</tr>
<tr>
<td>2-15</td>
<td>Configuration Interaction</td>
<td>10-20%</td>
</tr>
</tbody>
</table>

These methods cover all periodic system of elements.

They were used for many important problems:
- Test of Standard Model using Parity Violation in Cs, Tl, Pb, Bi
- Predicting spectrum of Fr (accuracy 0.1%), etc.
Results of calculations (in cm⁻¹)

<table>
<thead>
<tr>
<th>Atom</th>
<th>$\omega_0$</th>
<th>q</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg I</td>
<td>35051.217</td>
<td>86</td>
</tr>
<tr>
<td>Mg II</td>
<td>35760.848</td>
<td>211</td>
</tr>
<tr>
<td>Mg II</td>
<td>35669.298</td>
<td>120</td>
</tr>
<tr>
<td>Si II</td>
<td>55309.3365</td>
<td>520</td>
</tr>
<tr>
<td>Si II</td>
<td>65500.4492</td>
<td>50</td>
</tr>
<tr>
<td>Al II</td>
<td>59851.924</td>
<td>270</td>
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<tr>
<td>Al III</td>
<td>53916.540</td>
<td>464</td>
</tr>
<tr>
<td>Al III</td>
<td>53682.880</td>
<td>216</td>
</tr>
<tr>
<td>Ni II</td>
<td>58493.071</td>
<td>-20</td>
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</table>

Negative shifters

<table>
<thead>
<tr>
<th>Atom</th>
<th>$\omega_0$</th>
<th>q</th>
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<tbody>
<tr>
<td>Ni II</td>
<td>57420.013</td>
<td>-1400</td>
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<tr>
<td>Ni II</td>
<td>57080.373</td>
<td>-700</td>
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<td>Cr II</td>
<td>48632.055</td>
<td>-1110</td>
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<td>Cr II</td>
<td>48491.053</td>
<td>-1280</td>
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<tr>
<td>Cr II</td>
<td>48398.862</td>
<td>-1360</td>
</tr>
<tr>
<td>Fe II</td>
<td>62171.625</td>
<td>-1300</td>
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Positive shifters

<table>
<thead>
<tr>
<th>Atom</th>
<th>$\omega_0$</th>
<th>q</th>
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</thead>
<tbody>
<tr>
<td>Fe II</td>
<td>62065.528</td>
<td>1100</td>
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<td>Fe II</td>
<td>42658.2404</td>
<td>1210</td>
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<td>Fe II</td>
<td>42114.8329</td>
<td>1590</td>
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<tr>
<td>Fe II</td>
<td>41968.0642</td>
<td>1460</td>
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<tr>
<td>Fe II</td>
<td>38660.0494</td>
<td>1490</td>
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<tr>
<td>Fe II</td>
<td>38458.9871</td>
<td>1330</td>
</tr>
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<td>Zn II</td>
<td>49355.002</td>
<td>2490</td>
</tr>
<tr>
<td>Zn II</td>
<td>48841.077</td>
<td>1584</td>
</tr>
</tbody>
</table>

Also, many transitions in Mn II, Ti II, Si IV, C II, C IV, N V, O I, Ca I, Ca II, Ge II, O II, Pb II, Co II, ...

Different signs and magnitudes of q provides opportunity to study systematic errors!
Distance dependence

\( \Delta \alpha/\alpha = B \cos \Theta + m \) showing the gradient in \( \alpha \) along the best-fit dipole. The best-fit direction is at right ascension \( 17.4 \pm 0.6 \) hours, declination \( -62 \pm 6 \) degrees, for which \( B = (1.1 \pm 0.2) \times 10^{-6} \) GLyr\(^{-1} \) and \( m = (-1.9 \pm 0.8) \times 10^{-6} \). This dipole+monopole model is statistically preferred over a monopole-only model also at the 4.1\( \sigma \) level. A cosmology with parameters \((H_0, \Omega_M, \Omega_\Lambda) = (70.5, 0.2736, 0.726)\).
Keck & VLT dipoles independently agree, $p=4\%$
Low and high redshift cuts are consistent in direction. Effect is larger at high redshift.

$z > 1.6$

$z < 1.6$

Combined
Hints that this result might be real

Two internal consistencies:

1 Keck and VLT dipoles agree. Independent samples, different data reduction procedures, different instruments and telescopes.

2 High and low redshift dipoles also agree - different species used at low and high redshift – and different transitions respond differently to the same change in $\alpha$.

300 absorption systems, 30 atomic lines

Plank satellite Cosmic Microwave Background data 2013: Universe is not symmetric! CMB fluctuations are different in different directions.

Limits on dependence of alpha on gravity from white dwarf spectra Fe4+,Ni4+ 4.2(1.6) $10^{-5}$. Accurate laboratory spectra needed.
Variation of strong interaction

Grand unification suggests coefficient $R$

\[
\frac{\Delta \left( \frac{m}{\Lambda_{\text{QCD}}} \right)}{\frac{m}{\Lambda_{\text{QCD}}}} = R \frac{\Delta \alpha}{\alpha}
\]

1. Proton mass $M_p = 3 \Lambda_{\text{QCD}}$, measure $m_e / M_p$

2. Nuclear magnetic moments

\[
\mu = g e \hbar c / 4M_p c, \quad g = g \left( \frac{m_q}{\Lambda_{\text{QCD}}} \right)
\]

3. Nuclear energy levels and resonances
Dependence on quark mass

• Dimensionless parameter is $m_q/\Lambda_{QCD}$. It is convenient to assume $\Lambda_{QCD}=$const, i.e. measure $m_q$ in units of $\Lambda_{QCD}$

• $m_\pi$ is proportional to $(m_q\Lambda_{QCD})^{1/2}$
  $$\Delta m_\pi/m_\pi=0.5\Delta m_q/m_q$$

• Other meson and nucleon masses remains finite for $m_q=0$. $\Delta m/m=K \Delta m_q/m_q$

Argonne: $K$ are calculated for $p,n,\rho,\omega,\sigma$.

$$m_q = \frac{m_u + m_d}{2} \approx 4 \text{ M eV}$$
$$\Lambda_{QCD} = 220 \text{ M eV} \rightarrow K = 0.02 - 0.06$$

Strange quark mass $m_s = 120 \text{ M eV}$
Nuclear magnetic moments depend on $\pi$-meson mass $m_\pi$

Nucleon magnetic moment

Spin-spin interaction between valence and core nucleons
Nucleon magnetic moment

\[ \mu = \mu_0 (1 + a m_\pi + ...) = \mu_0 (1 + b \sqrt{m_q} + ...) \]

Nucleon and meson masses

\[ M = M_0 + a m_q \]

QCD calculations: lattice, chiral perturbation theory, cloudy bag model, Dyson-Schwinger and Faddeev equations, semiempirical.

Nuclear calculations: meson exchange theory of strong interaction. Nucleon mass in kinetic energy \( \frac{p^2}{2M} \)
\( m_e / M_p \) limit from \( \text{NH}_3 \)

Inversion spectrum: exponentially small “quantum tunneling” frequency
\[
\omega_{\text{inv}} = W \exp(-S(m_e / M_p))
\]
\( \omega_{\text{inv}} \) is exponentially sensitive to \( m_e / M_p \)
Laboratory measurements proposed (Veldhoven et al)

Astrophysics - \(-2\) systems containing \( \text{NH}_3 \)
Flambaum, Kozlov  PRL 2007
First enhanced effect in quasar spectra
\[
\Delta(m_e / M_p) / (m_e / M_p) = -0.6(1.9)10^{-6} \text{ No variation}
\]
z=0.68, 6.5 billion years ago, -1(3)10^{-16} /year

More accurate measurements
Murphy, Flambaum, Henkel, Muller.  Science 2008  -0.74(0.47)(0.76)10^{-6}
Henkel et al AA 2009  z=0.87  <1.4 10^{-6}  3 \sigma

Levshakov, Molaro, Kozlov 2008 our Galaxy 0.5(0.14)10^{-7}
Metanol
Hydrogen molecule - 4 systems

\[ \Delta \left( \frac{m_e}{M_p} \right) / \left( \frac{m_e}{M_p} \right) = 3.3(1.5) \times 10^{-6} \ r \cos(\phi) \]

gradient direction \( 16.7(1.5) \ h, -62(5)^\circ \)
consistent with \( \alpha \) gradient direction
\( 17.6(0.6) \ h, -58(6)^\circ \)

If we assume the same direction
\[ 2.6(1.3) \times 10^{-6} \ r \cos(\phi) \quad 4\% \ by \ chance \]
Big Bang nucleosynthesis: dependence on quark mass

- Flambaum, Shuryak 2002
- Flambaum, Shuryak 2003
- Dmitriev, Flambaum 2003
- Dmitriev, Flambaum, Webb 2004
- Coc, Nunes, Olive, Uzan, Vangioni 2007
- Dent, Stern, Wetterich 2007
- Flambaum, Wiringa 2007
- Berengut, Dmitriev, Flambaum 2010
- Bedaque, Luu, Platter 2011
- Berengut, Eppelbaum, Flambaum, Hanhart, Meissner, Nebreda, Pelaez 2013
Deutron binding energy is sensitive to the variation of the quark mass

- Shallow level: small variation of the potential leads to large variation of the binding energy.
- Virtual level in (n+p) is even more sensitive, and it influences the deuterium formation rate.
- BBN is exponentially sensitive to the deuteron binding energy $E$, $\exp(-E/T)$
Deuterium abundance – 7 points

Big Bang Nucleosynthesis data give direction of the gradient in the deuterium abundance consistent with the direction of the $\alpha$ gradient. However, the amplitude of the relative spatial variation $0.0045(35)$ is not statistically significant. This would result in relative variation of $X = m_q / \Lambda_{QCD}$

$$\Delta X/X = 0.0013(10) \ r \cos(\phi)$$

$$\Delta \alpha/\alpha = 0.003(3) \ r \cos(\phi)$$

Compare with QSO

$$\Delta \alpha/\alpha = 1.10(0.25) \times 10^{-6} \ r \cos(\phi)$$
Gradient $\alpha$ points down
Oklo natural nuclear reactor

$n^{+149}\text{Sm}$ capture cross section is dominated by $E_r = 0.1$ eV resonance. Shlyakhter-limit on $\Delta\alpha/\alpha$ two billion years ago

Our QCD/nuclear calculations

$\Delta E_r = 10 \text{ MeV} \Delta X_q/X_q - 1 \text{ MeV} \Delta\alpha/\alpha$

$X_q = m_q/\Lambda_{\text{QCD}}$, enhancement $10 \text{ MeV}/0.1 \text{ eV} = 10^8$

Galaxy moves 552 km/s relative to CMB, $\cos(\phi) = 0.23$

Dipole in space: $\Delta E_r = (10 R - 1) \text{ meV}$

Fujii et al $|\Delta E_r| < 20 \text{ MeV}$

Gould et al, $-12 < \Delta E_r < 26 \text{ meV}$

Petrov et al $-73 < \Delta E_r < 62 \text{ meV}$
Consequences for atomic clocks

• Sun moves 369 km/s relative to CMB 
  \( \cos(\phi) = 0.1 \)
  This gives average laboratory variation
  \( \frac{\Delta \alpha}{\alpha} = 1.5 \times 10^{-18} \cos(\phi) \) per year

• Earth moves 30 km/s relative to Sun-
  \( 1.6 \times 10^{-20} \cos(\omega t) \) annual modulation
Atomic clocks:

Comparing rates of different clocks over long period of time can be used to study time variation of fundamental constants

Optical transitions: \( \alpha \)

Microwave transitions: \( \alpha, \left( m_e, m_q \right) / \Lambda_{QCD} \)
Calculations to link change of frequency to change of fundamental constants:

Optical transitions: **atomic calculations** (as for quasar absorption spectra) for many narrow lines in Al II, Ca I, Sr I, Sr II, In II, Ba II, Dy I, Yb I, Yb II, Yb III, Hg I, Hg II, Tl II, Ra II, Th IV

\[ \omega = \omega_0 + q\left( \frac{\alpha^2}{\alpha_0^2} - 1 \right) \]

Microwave transitions: hyperfine frequency is sensitive to nuclear magnetic moments and nuclear radii

We performed atomic, nuclear and QCD calculations of powers \( \kappa, \beta \) for H, D, Rb, Cd\(^+\), Cs, Yb\(^+\), Hg\(^+\)

\[ V = C(\text{Ry})(m_e/M_p)\alpha^{2+\kappa}(m_q/\Lambda_{\text{QCD}})^{\beta}, \Delta \omega/\omega = \Delta V/V \]

Cs: \( \beta = 0 \), \( m_e/M_p \) measurement! Not magnetic moment.

Rydberg constant in SI units = Cs hyperfine = \((m_e/M_p)^{2.83}\)
We performed atomic, nuclear and QCD calculations of powers $\kappa, \beta$ for H, D, He, Rb, Cd$^+$, Cs, Yb$^+$, Hg$^+$...

$$V = C(Ry)(m_e/M_p)\alpha^{2+\kappa} (m_q/\Lambda_{QCD})^\beta, \quad \Delta \omega/\omega = \Delta V/V$$

$^{133}\text{Cs}$: $\kappa = 0.83, \beta = 0.002$

Cs standard is insensitive to variation of $m_q/\Lambda_{QCD}$!

$^{87}\text{Rb}$: $\kappa = 0.34, \beta = -0.02$

$^{171}\text{Yb}^+$: $\kappa = 1.5, \beta = -0.10$

$^{199}\text{Hg}^+$: $\kappa = 2.28, \beta = -0.11$

$^1\text{H}$: $\kappa = 0, \beta = -0.10$

## Results for variation of fundamental constants

<table>
<thead>
<tr>
<th>Source</th>
<th>Clock$_1$/Clock$_2$</th>
<th>$d\alpha/\alpha(10^{-16}$ yr$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blatt et al, 2007</td>
<td>Sr(opt)/Cs(hfs)</td>
<td>-3.1(3.0)</td>
</tr>
<tr>
<td>Fortier et al 2007</td>
<td>Hg+(opt)/Cs(hfs)</td>
<td>-0.6(0.7)$^a$</td>
</tr>
<tr>
<td>Rosenband et al 2008</td>
<td>Hg+(opt)/Al+(opt)</td>
<td>-0.16(0.23)</td>
</tr>
<tr>
<td>Peik et al, 2006</td>
<td>Yb+(opt)/Cs(hfs)</td>
<td>4(7)</td>
</tr>
<tr>
<td>Guena et al, 2012</td>
<td>Rb(hfs)/Cs(hfs)</td>
<td>3(2)$^a$</td>
</tr>
</tbody>
</table>

$^a$assuming $m_{q,e}/\Lambda_{QCD} =$ Const

**Combined results:**

\[
\frac{d}{dt} \ln \alpha = -1.6(2.3) \times 10^{-17} \text{ yr}^{-1}
\]

\[
\frac{d}{dt} \ln \left( \frac{m_q}{\Lambda_{QCD}} \right) = 7(4) \times 10^{-15} \text{ yr}^{-1}
\]

\[
\frac{m_e}{M_p} \text{ or } \frac{m_e}{\Lambda_{QCD}} = -1.5(3.0) \times 10^{-16} \text{ yr}^{-1}
\]
Largest $q$ in multiply charged ions, narrow lines

$q$ increases as $Z^2(Z_i+1)^2$

To keep frequencies in optical range we use configuration crossing as a function of $Z$. Projected accuracy $10^{-19}$

Crossing of 5f and 7s

Th IV: $q_1 = -75300$

Crossing of 4f and 5s

Sm15+, Pm14+, Nd 13+

Difference $q = q_2 - q_1$ is 260 000

5 times larger than in Hg II/Al II

Relative enhancement up to 500

In Sm+14 there are narrow transitions and E1 transitions in the laser range, for cooling,

Holes in filled shells: 13 times larger $q$ than in Hg II/Al II

Cf: 23 times larger than in Hg II/Al II

New accurate calculations of energy levels and electromagnetic amplitudes
Atomic clocks with highly charged ions

Highly charged ions have small size, \( r = \text{const} / Z_{\text{ion}} \)

Narrow E2 transitions, \( r^2 \)

Greatly reduced coupling to external perturbations:
Polarizability \( r^3 \)
Small black body radiation shift
Suppressed quadrupole shift, etc

Precision at the level \( 10^{-19} \)

Derevianko, Dzuba, Flambaum 2012; Berengut, Dzuba, Flambaum, Ong 2012

Plus enhanced sensitivity to \( \alpha \) variation: potential for 2-3 order of magnitude improvement in laboratory measurements of \( \alpha \) variation
Enhancement of relative effect

Our proposal and calculations:

Dy: \(4f^{10}5d6s\) E=19797.96... cm\(^{-1}\), q= 6000 cm\(^{-1}\)
\(4f^95d^26s\) E=19797.96... cm\(^{-1}\), q= -23000 cm\(^{-1}\)

\(\omega_0 = 10^{-4} \text{ cm}^{-1}\). Relative enhancement \(\Delta \omega/\omega_0 = 10^8 \Delta \alpha/\alpha\)

Measurement Berkeley \(d\ln \alpha/dt = -6(7) \times 10^{-17} \text{ yr}^{-1}\)

Different signs of \(\omega_0\) in different isotopes: cancellation of errors!

Limits on dependence of \(\alpha\) on gravity, Lorentz invariance and equivalence principle violation, parity violation

Close narrow levels in molecules
Nuclear clocks

Peik, Tamm 2003: UV transition between first excited and ground state in $^{229}\text{Th}$ nucleus. Energy $7.6(5)$ eV, width $10^{-3}$ Hz. Perfect clock!

We made specific clock proposals: Th+, Th+3. Projected accuracy $10^{-19}$

Flambaum 2006: Nuclear/QCD estimate- Enhancement $10^5$

He, Re; Flambaum, Wiringa; Flambaum, Auerbach, Dmitriev; Hayes, Friar, Moller; Litvinova, Feldmeier, Dobaczewski, Flambaum;

$\Delta \omega = 10^{19}$ Hz ($\Delta \alpha/\alpha + 10 \Delta X_q/X_q$), $X_q = m_q/\Lambda_{QCD}$

Shift 10-100 Hz for $\Delta \alpha/\alpha=10^{-18}$

Compare with atomic clock shift 0.001 Hz

Enhancement is due to cancellation of large contributions of strong and electromagnetic interactions, $\omega = S+Q=100$ KeV-100 KeV

$^{235}\text{U}$ nucleus, 76 eV transition, laser build by Jun Ye group.

Variation effect is larger than in $^{229}\text{Th}$
Dependence on $\alpha$

$$\Delta \omega = Q \frac{\Delta \alpha}{\alpha}$$

- Total Coulomb energy $10^9$ eV in $^{229}$Th
- Difference of moments of inertia between ground and excited states is 4% (?)
- If difference in the Coulomb energy would be 0.01%, $Q=100$ KeV, estimate for the enhancement factor

$$\frac{Q}{\omega_0} = 10^5 \text{ eV} / 7 \text{ eV} = 1.4 \times 10^4$$
Sensitivity to $\Delta \alpha$ may be obtained from measurements

$$\Delta \omega = Q \frac{\Delta \alpha}{\alpha}$$

Berengut, Dzuba, Flambaum, Porsev PRL 2009

$Q/\text{Mev} = -506 \frac{\Delta \langle r^2 \rangle}{\langle r^2 \rangle} + 23 \frac{\Delta Q_2}{Q_2}$

Difference of squared charge radii $\Delta \langle r^2 \rangle$ may be extracted from isomeric shifts of electronic transitions in Th atom or ions

Difference of electric quadrupole moments $\Delta Q_2$ from hyperfine structure
$^{229}\text{Th}: \text{Flambaum, Wiringa 2007}$

Sensitivity to quark mass

$\omega = E_{pk} + E_{so} + Q = 7.6 \text{ eV}$ \text{ huge cancellations!}

$E_{so} = <V_s L S> = \text{spin-orbit} = -1.04 \text{ MeV}$

$E_{pk} = \text{potential+kinetic} = 1 \text{ MeV}$

Extrapolation from light nuclei

$\Delta E_{pk}/E_{pk} = -1.4 \Delta m_q/m_q$

$\Delta E_{so}/E_{so} = -0.24 \Delta m_q/m_q$

$\Delta \omega/\omega_0 = 1.6 \times 10^5 \Delta X_q/X_q$
Nuclear clocks $^{229}$Th3+: 19 digits precision

In stretched states $F = F_z = l_{\text{nucleus}} + l_{\text{electron}}$ the ion wave function is a product of electron and nuclear wave functions. Electronic shifts produced by external perturbations in the ground and excited nuclear states are equal and cancel out.

Nuclear size is very small. Nuclear polarizability, black body radiation shift and other shifts are very small.

Campbell, Radnaev, Kuzmich, Dzuba, Flambaum, Derevianko PRL 2012

Potential to improve sensitivity to variation of the fundamental constants by 7 orders of magnitude
Electron bridge mechanism to excite nuclear transitions

Excitation of atomic electrons which transfer energy to nucleus.

Calculations in Th+ and Th3+
Th3+ Porsev, Flambaum PRA 2010, PRA 2010
Th+ Porsev, Flambaum, Peik, Tamm PRL 2010

Exponential increase of energy level density in atoms: Th ,Th+. Dzuba, Flambaum PRL2010

Close nuclear and atomic energy levels
Conclusions

• Spatial gradient of alpha from quasar data, 4.2 sigma, Keck and VLT data agree, low and high red shift data agree, no contradictions with other groups.

• It provides alpha variation for atomic clocks due to Earth motion at the level $10^{-18}$ and 1 meV shift in Oklo resonance. One-two orders of magnitude improvement in the measurement accuracy is needed. Three orders for meteorites.

• Very weak indications for the spatial variation in H$_2$ quasar spectra and BBN abundance of deuterium. The same direction of the gradient!

New systems with higher absolute sensitivity include:

• transitions between ground and metastable states in highly charged ions. Frequencies are kept in laser spectroscopy range due to the configuration crossing phenomenon. An order of magnitude gain.

• $^{229}$Th nucleus – highest absolute enhancement (10$^5$ times larger shift), UV transition 7eV.

• Many systems with relative enhancement due to transition between close levels: Dy atom, a number of molecules with narrow close levels,…

• Search for anisotropy in CMB, expansion of the Universe, structure formation
Parity and time reversal violation in atoms, molecules and nuclei and search for physics beyond the Standard Model

Victor Flambaum

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Atomic parity violation

• Dominated by Z-boson exchange between electrons and nucleons

\[ H = \frac{G}{\sqrt{2}} \left[ C_{1p} \bar{e} \gamma_\mu \gamma_5 e \bar{p} \gamma^\mu p + C_{1n} \bar{e} \gamma_\mu \gamma_5 e \bar{n} \gamma^\mu n \right] \]

Standard model

• In atom with Z electrons and N neutrons obtain effective Hamiltonian parameterized by “nuclear weak charge” \( Q_W \)

\[ h_{PV} = \frac{G}{2\sqrt{2}} Q_W \rho(r) \gamma_5 \]

\[ Q_W = 2(NC_{1n} + ZX_{1p}) \approx -N + Z(1 - 4\sin^2 \theta_W) \approx -N \]

• PV amplitude \( E_{PV} \propto Z^3 \) [Bouchiat,Bouchiat]

Discovered in 1978 Bi; Tl, Pb, Cs –accuracy 0.4-1%  
Our calculations in 1975-1989 Bi 11%, Pb 8%, Tl 3%, Cs 1%
Cs: accuracy of experiment and theory 0.4%, agreement with the standard model, limits on new physics. Calculations and experiments in Cs analogues Our calculations and calculations of other groups

Ba+

Fr, Ra+, Ac+2, Th+3  PNC effects 15 times larger

Experiments in Seattle (Ba+), TRIUMF (Fr), Groningen (Ra+)
PV : Chain of isotopes

Dzuba, Flambaum, Khriplovich

Rare-earth atoms:
• close opposite parity levels-enhancement
• Many stable isotopes

Ratio of PV effects gives ratio of weak charges. Uncertainty in atomic calculations cancels out. Experiments:
Berkeley: Dy and Yb; PV amplitude 100 x Cs!
Ra\(^+\) - Groningen, Fr- TRIUMF

Fortson, Pang, Wilets Test of Standard model or neutron distribution?

Brown, Derevianko, Flambaum 2009. Uncertainties in neutron distributions cancel in differences of PV effects in isotopes of the same element. **Measurements of ratios of PV effects in isotopic chain can compete with other tests of Standard model!**
Nuclear anapole moment

- Source of nuclear spin-dependent PV effects in atoms
- Nuclear magnetic multipole violating parity
- Arises due to parity violation inside the nucleus

- Interacts with atomic electrons via usual magnetic interaction (PV hyperfine interaction):

$$\hat{\mathbf{a}} = e \alpha \cdot \mathbf{A} \propto \kappa_a \alpha \cdot \mathbf{I} \rho(r), \quad \kappa_a \propto A^{2/3}$$

[Flambaum, Khriplovich, Sushkov]

$$E_{PV} \propto Z^2 A^{2/3}$$ measured as difference of PV effects for transitions between hyperfine components

Cs: $|6s, F=3\rangle - |7s, F'=4\rangle$ and $|6s, F'=4\rangle - |7s, F=3\rangle$

Probe of weak nuclear forces via atomic experiments!
Nuclear anapole moment is produced by PV nuclear forces. Measurements and our calculations give the strength constant $g$.

- Boulder Cs: $g=6(1)$ in units of Fermi constant
- Seattle Tl: $g=-2(3)$

New accurate calculations Flambaum, Hanhart; Haxton, Liu, Ramsey-Musolf; Auerbach, Brown; Dmitriev, Khriplovich, Telitsin: problem remains.

Experiments and proposals: Fr (TRIUMF), $10^3$ enhancement in Ra atom due to close opposite parity state; Dy, Yb, ... (Berkeley)
Enhancement of nuclear anapole effects in molecules

$10^5$ enhancement of the anapole contribution in diatomic molecules due to mixing of close rotational levels of opposite parity. Theorem: only nuclear-spin-dependent (anapole) contribution to PV is enhanced (Labzovsky; Sushkov; Flambaum 1978). Weak charge can not mix opposite parity rotational levels and $\Lambda$–doublet.

$\Omega=1/2$ terms: $\Sigma_{1/2}$, $\Pi_{1/2}$. Heavy molecules, effect $Z^2 A^{2/3} R(Z\alpha)$

YbF, BaF, PbF, LuS, LuO, LaS, LaO, HgF, ... Cl, Br, I, ... BiO, BiS, ...

Cancellation between hyperfine and rotational intervals-enhancement. Interval between the opposite parity levels may be reduced to zero by magnetic field – further enhancement.

Molecular experiments: Yale, Groningen, NWU.

New calculations for many molecules and molecular ions:
  Borschevsky, Ilias, Beloy, Dzuba, Flambaum, Schwerdtfeger 2012
Accurate molecular calculations and proposals by other groups

• RaF: T.A.Isaev, S. Hoekstra, R.Berger.
• BaF: M.G.Kozlov, A,V.Titov, N.S. Mosyagin, P.V. Souchko. M.N.Nayak, B. Das, ...

Experimental proposals:

• DeMille et al
• T.A.Isaev, S. Hoekstra, R. Berger.
Atomic electric dipole moments

- Electric dipole moments violate parity (P) and time-reversal (T)

- \( T \)-violation \( \equiv \) CP-violation by CPT theorem

**CP violation**

- Observed in \( \Lambda^0 \), \( B^0 \)
- Accommodated in SM as a single phase in the quark-mixing matrix (Kobayashi-Maskawa mechanism)

However, not enough CP-violation in SM to generate enough matter-antimatter asymmetry of Universe!

\( \Rightarrow \) Must be some non-SM CP-violation
• Excellent way to search for new sources of CP-violation is by measuring EDMs

  - SM EDMs are hugely suppressed

  → Theories that go beyond the SM predict EDMs that are many orders of magnitude larger!

* e.g. electron EDM

<table>
<thead>
<tr>
<th>Theory</th>
<th>$d_e$ (e cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Std. Mdl.</td>
<td>&lt; $10^{-38}$</td>
</tr>
<tr>
<td>SUSY</td>
<td>$10^{-28}$ - $10^{-26}$</td>
</tr>
<tr>
<td>Multi-Higgs</td>
<td>$10^{-28}$ - $10^{-26}$</td>
</tr>
<tr>
<td>Left-right</td>
<td>$10^{-28}$ - $10^{-26}$</td>
</tr>
</tbody>
</table>

**Best limit (90% c.l.):** $|d_e| < 1.6 \times 10^{-27}$ e cm

Berkeley (2002)

• Atomic EDMs $d_{\text{atom}} \propto Z^3$  

  [Sandars]  

  Sensitive probe of physics beyond the Standard Model!
Atomic EDMs

Best limits

$|d^{(199}\text{Hg})| < 3 \times 10^{-29} \text{ e cm}$
(95% c.l., Seattle, 2009)

$|d^{(205}\text{Tl})| < 9.6 \times 10^{-25} \text{ e cm}$
(90% c.l., Berkeley, 2002)
YbF, London 2012

$|d(n)| < 2.9 \times 10^{-26} \text{ e cm}$
(90% c.l., Grenoble, 2006)

Leading mechanisms for EDM generation

fundamental CP-violating phases

$\theta_{qq}$

neutron EDM

$|d-\text{el}|$

$\text{EDMs of diamagnetic systems (Hg,Ra)}$

$\text{EDMs of paramagnetic systems (Tl)}$

Leading mechanisms for EDM generation

$\psi = + + -$

$\psi^2 = -$
Nuclear EDM:
T,P-odd NN interaction gives 40 times larger contribution than nucleon EDM
Sushkov, Flambaum, Khriplovich 1984
T,P-odd NN interaction

Khriplovich, Sushkov, Flambaum 1984,1986
• Calculations of nuclear EDM and Schiff moments
• Calculations of atomic EDM
• Calculation of T,P-odd \( \pi \) NN and nucleon-nucleon interaction in the Standard model. NN interaction strength 0.3 \( 10^{-8} \) G. Current limit from atomic EDM \( 10^{-4} \) G.
• We need physics beyond Standard model
• Or new enhanced effects.
Nuclear EDM-screening: $d_N E_N$

- Schiff theorem: $E_N = 0$, neutral systems
- Extension for ions and molecules: Flambaum, Kozlov

Ion acceleration $a = Z_i eE/M$
Nucleus acceleration $a = Z eE_N/M$

$$E_N = E \frac{Z_i}{Z}$$

In molecules screening is stronger:

$$a = Z_i eE/(M+m), \quad E_N = E \left(\frac{Z_i}{Z}\right)\left(\frac{M}{(M+m)}\right)$$

Schiff moment dominates in molecules!
Diamagnetic atoms and molecules

Source-nuclear Schiff moment

SM appears when screening of external electric field by atomic electrons is taken into account.

Nuclear T,P-odd moments:

• EDM – non-observable due to total screening (Schiff theorem)

Nuclear electrostatic potential with screening (our 1984 calculation following ideas of Schiff and Sandars):

$$
\varphi(R) = \int \frac{e \rho(r)}{|R - r|} \, d^3r + \frac{1}{Z} (\mathbf{d} \cdot \nabla) \int \frac{\rho(r)}{|R - r|} \, d^3r
$$

$\mathbf{d}$ is nuclear EDM, the term with $\mathbf{d}$ is the electron screening term

$\varphi(R)$ in multipole expansion is reduced to

$$
\varphi(R) = 4\pi \mathbf{S} \cdot \nabla \delta(R)
$$

where

$$
\mathbf{S} = \frac{e}{10} \left[ \langle r^2 r \rangle - \frac{5}{3Z} \langle r^2 \rangle \rangle \right]
$$

is Schiff moment.

This expression is not suitable for relativistic calculations.
Flambaum, Ginges: 
$L = S(1 - \alpha Z^2)$

\[ \phi(R) = -\frac{3L \cdot R}{B} \rho(R) \]

where \[ B = \int \rho(R) R^4 dR \]

This potential has no singularities and may be used in relativistic calculations. SM electric field polarizes atom and produces EDM.


Atomic EDM: Sushkov, Flambaum, Khriplovich; Dzuba, Flambaum, Ginges, Kozlov.

Best limits from Hg EDM measurement in Seattle - Crucial test of modern theories of CP violation (supersymmetry, etc.)
Atomic EDM induced by Schiff moment rapidly increases with nuclear charge, $Z^2 R(Z^\alpha)$

- We performed accurate many-body calculations for heavy atoms: Xe, Yb, Hg, Rn, Ra; Measurements for Xe (Seattle, Ann Arbor) and Hg (Seattle).

- In molecules there is an additional enhancement suggested by Sandars: internal electric field of polarised molecule is orders of magnitude larger than applied external field

Calculations and measurements in TIF (Hinds)
Enhancement in nuclei with quadrupole deformation

Close level of opposite parity

- Haxton, Henley –EDM, MQM
- Sushkov, Flambaum, Khriplovich –Schiff moment
- Flambaum - spin hedgehog and collective magnetic quadrupole are produced by T,P-odd interaction which polarises spins along radius

Enhancement factor does not exceed 10
Nuclear enhancement
Auerbach, Flambaum, Spevak 1996

The strongest enhancement is due to octupole deformation (Rn,Ra,Fr,...)

\[ S_{\text{intr}} \approx eZR^3_N \frac{9 \beta_2 \beta_3}{20\pi \sqrt{35}} \]

\[ \beta_2 \approx 0.2 \quad \text{- quadrupole deformation} \]

\[ \beta_3 \approx 0.1 \quad \text{- octupole deformation} \]

No T,P-odd forces are needed for the Schiff moment and EDM in intrinsic reference frame
However, in laboratory frame \( S=d=0 \) due to rotation
In the absence of $T,P$-odd forces: doublet (+) and (-)

$$\Psi = \frac{1}{\sqrt{2}} \left( |IMK\rangle + |IM - K\rangle \right)$$

and $\langle n \rangle = 0$

$T,P$-odd mixing ($\beta$) with opposite parity state (-) of doublet:

$$\Psi = \frac{1}{\sqrt{2}} \left[ (1 + \beta)|IMK\rangle + (1 - \beta)|IM - K\rangle \right]$$

and $\langle n \rangle \propto |\beta|$

EDM and Schiff moment

$\langle d \rangle, \langle S \rangle \propto \langle n \rangle \propto |\beta|$
Simple estimate (Auerbach, Flambaum, Spevak):

\[ S_{\text{lab}} \propto \frac{\langle + | H_{TP} | - \rangle}{E_+ - E_-} S_{\text{body}} \]

Two factors of enhancement:
1. Large collective moment in the body frame
2. Small energy interval \((E_+ - E_-)\), 0.05 \text{eV} instead of 8 MeV

\[ S \approx 0.05 e \beta_2 \beta_3 Z A^{2/3} \eta r_0^3 \frac{\text{eV}}{E_+ - E_-} \approx 700 \times 10^{-8} \eta \text{efm}^3 \approx 500 S(\text{Hg}) \]

\(^{225}\text{Ra}, ^{223}\text{Rn}, \text{Fr, ...} \quad -100-1000 \text{ times enhancement} \)
Engel, Friar, Hayes (2000); Flambaum, Zelevinsky (2003):
Static octupole deformation is not essential, nuclei with soft octupole vibrations also have the enhancement.
Nature 2013 Measurements of octupole deformation
# EDMs of atoms of experimental interest

<table>
<thead>
<tr>
<th>Z</th>
<th>Atom</th>
<th>([S/(e \text{ fm}^3)]e\ \text{ cm})</th>
<th>([10^{-25} \eta]e\ \text{ cm})</th>
<th>Expt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>(^3\text{He})</td>
<td>0.00008</td>
<td>0.0005</td>
<td></td>
</tr>
<tr>
<td>54</td>
<td>(^{129}\text{Xe})</td>
<td>0.38</td>
<td>0.7</td>
<td>Seattle, Ann Arbor, Princeton</td>
</tr>
<tr>
<td>70</td>
<td>(^{171}\text{Yb})</td>
<td>-1.9</td>
<td>3</td>
<td>Bangalore, Kyoto</td>
</tr>
<tr>
<td>80</td>
<td>(^{199}\text{Hg})</td>
<td>-2.8</td>
<td>4</td>
<td>Seattle</td>
</tr>
<tr>
<td>86</td>
<td>(^{223}\text{Rn})</td>
<td>3.3</td>
<td>3300</td>
<td>TRIUMF</td>
</tr>
<tr>
<td>88</td>
<td>(^{225}\text{Ra})</td>
<td>-8.2</td>
<td>2500</td>
<td>Argonne, KVI</td>
</tr>
<tr>
<td>88</td>
<td>(^{223}\text{Ra})</td>
<td>-8.2</td>
<td>3400</td>
<td></td>
</tr>
</tbody>
</table>

Standard Model \(\eta = 0.3 \times 10^{-8}\) \(\quad d_n = 5 \times 10^{-24} e\ \text{ cm} \ \eta, \quad d(^{199}\text{Hg})/d_n = 10^{-1}\)
RaO molecule

Enhancement factors

• Biggest Schiff moment
• Highest nuclear charge
• Close rotational levels of opposite parity (strong internal electric field)

Largest T,P-odd nuclear spin-axis interaction $\kappa(I,n)$, RaO= 200 TIF

Flambaum 2008; Kudashov, Petrov, Skripnikov, Mosyagin, Titov, Flambaum 2013
Sandars: Enhancement of electron EDM in heavy atoms and molecules

• Flambaum: Atomic enhancement = $3Z^3 \alpha^2 R(Z\alpha)$

Tl enhancement $d(\text{Tl}) = -585 \, d_e$

Experiment – Berkeley

• Sushkov, Flambaum 1978 Molecules – close rotational levels, additional enhancement $M/m_e$

$\Omega$ – doubling – huge enhancement of electron EDM

$\Omega = 1/2 \quad 10^7 \quad \text{YbF} \quad \text{London}$

$\Omega = 1 \quad 10^{10} \quad \text{PbO} \quad \text{Yale}$

$\text{HfF}^+ \quad \text{Boulder}$

$\text{ThO} \quad \text{Harvard, Yale}$

Weak electric field is enough to polarise the molecule. Molecular electric field is several orders of magnitude larger than external field (Sandars). Accurate calculations available.
Extra enhancement in excited states: Ra

\[ d_{\text{atom}} (1) = 2 \sum_{N} \frac{\langle 1 | D_z | N \rangle \langle N | H_{PT} | 1 \rangle}{E_1 - E_N} \]

- Extra enhancement for EDM and APV in metastable states due to presence of close opposite parity levels
  [Flambaum; Dzuba,Flambaum,Ginges]

\[ d(3D_2) \sim 10^5 \times d(\text{Hg}) \]

\[ E_{PV}(1S_0-3D_{1,2}) \sim 100 \times E_{PV}(\text{Cs}) \]

Comparison of even Ra isotopes

anapole moment: \[ \sim 10^3 E_{PV} (\text{Cs}) \]

Strongly enhanced data
Summary

- Atomic and molecular experiments are used to test unification theories of elementary particles

Parity violation
- Weak charge: test of the standard model and search of new physics
- Chain of isotopes method can compete with other methods to search for physics beyond the Standard model and measure difference of neutron skins
- Nuclear anapole, probe of weak PV nuclear forces

Time reversal
- EDM, test of physics beyond the standard model.
  1-3 orders improvement may be enough to reject or confirm all popular models of CP violation, e.g. supersymmetric models

- A new generation of experiments with enhanced effects is underway in atoms, diatomic molecules, and solids