"We feel clearly that we are only now beginning to acquire reliable material for welding together the sum total of all that is known into a whole, but, on the other hand, it has become next to impossible for a single mind fully to command more than a small specialized portion of it. I can see no other escape from this dilemma (lest our true aim be lost forever) than that some of us should venture to embark on a synthesis of facts and theories, albeit with second-hand and incomplete knowledge of them - and at the risk of making fools of ourselves."

Marsden Fund NZ, Alexander von Humboldt Foundation
Toward the Theory of Everything

- Gravitational force
  - General Relativity
- Strong force
  - SU(3)
  - Quantum Chromodynamics
  - SU(3) \times U(1)
- Electromagnetic force
  - U(1)
  - Quantum Electrodynamics
  - SU(2) 
  - Electrodynamics
- Weak force
  - SU(2) \times U(1)
  - Electroweak Theory
  - GUT
- SU(3) \times SU(2) \times U(1)
  - Standard Model
  - String-Theory
  - SUSY
One fundamental particle predicted by the SM yet to be discovered

Peter Higgs and the Higgs boson (~126 GeV)

<table>
<thead>
<tr>
<th>Quarks</th>
<th>Mass (MeV)</th>
<th>Charge</th>
<th>Spin</th>
<th>Name</th>
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<tr>
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<tr>
<td>gluon (g)</td>
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<td>muon neutrino (ν_μ)</td>
<td>&lt;0.17</td>
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<tr>
<td>tau neutrino (ν_τ)</td>
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<tr>
<td>Z^0 weak force</td>
<td>91.2</td>
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<tr>
<td>W^± weak force</td>
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<th>Charge</th>
<th>Spin</th>
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<tr>
<td>electron (e)</td>
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<tr>
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<tr>
<td>weak force</td>
<td>80.4</td>
<td>±1</td>
<td>±1</td>
<td>80.4</td>
<td>1</td>
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</table>
Lagrangian of the Standard Model

\[ \mathcal{L} = -\frac{1}{4} B_{\mu\nu} B^{\mu\nu} - \frac{1}{8} \text{tr}(W_{\mu\nu} W^{\mu\nu}) - \frac{1}{2} \text{tr}(G_{\mu\nu} G^{\mu\nu}) \]

\[ + (\bar{\nu}_L, \bar{e}_L) \tilde{\sigma}^\mu i D_\mu \left( \begin{array}{c} \nu_L \\ e_L \end{array} \right) + \bar{e}_R \sigma^\mu i D_\mu e_R + \bar{\nu}_R \sigma^\mu i D_\mu \nu_R \]

\[ - \frac{\sqrt{2}}{v} \left[ (\bar{\nu}_L, \bar{e}_L) \phi M^e e_R + \bar{e}_R M^{e*} \phi \left( \begin{array}{c} \nu_L \\ e_L \end{array} \right) \right] \]

\[ - \frac{\sqrt{2}}{v} \left[ (-\bar{e}_L, \bar{\nu}_L) \phi^* M^\nu \nu_R + \bar{\nu}_R M^{\nu*} \phi^T \left( \begin{array}{c} -e_L \\ \nu_L \end{array} \right) \right] \]

\[ + (\bar{u}_L, \bar{d}_L) \tilde{\sigma}^\mu i D_\mu \left( \begin{array}{c} u_L \\ d_L \end{array} \right) + \bar{u}_R \sigma^\mu i D_\mu u_R + \bar{d}_R \sigma^\mu i D_\mu d_R \]

\[ - \frac{\sqrt{2}}{v} \left[ (\bar{u}_L, \bar{d}_L) \phi M^d d_R + \bar{d}_R M^{d*} \phi \left( \begin{array}{c} u_L \\ d_L \end{array} \right) \right] \]

\[ - \frac{\sqrt{2}}{v} \left[ (-\bar{d}_L, \bar{u}_L) \phi^* M^u u_R + \bar{u}_R M^{u*} \phi^T \left( \begin{array}{c} -d_L \\ u_L \end{array} \right) \right] \]

\[ + (D_\mu \bar{\phi}) D^\mu \phi - m_h^2 [\bar{\phi} \phi - v^2/2]^2/\nu^2, \]

\[ + \text{(Hermitian conjugate of some terms).} \]

QED

For every complex problem there is an answer that is clear, simple, and wrong.

Henry Louis Mencken
Richard Feynman: So far we have found nothing wrong with QED. It is, therefore, the jewel of physics – our proudest possession.

Precision tests of QED consist of the accurate determination of the **electromagnetic fine structure constant** $\alpha$ (esu)

$$\alpha^{-1} = \frac{hc}{e^2} = 137.035999676(94)$$

The most precise determination of the fine-structure constant $\alpha$ comes from the electron **$g$-factor**. The intrinsic spin of the electron produces a magnetic moment

$$\vec{\mu} = g_e \frac{e\hbar}{2m_e c} \hat{s} \quad , \quad g_e = g_e = \begin{cases} 1 & \text{classical} \\ 2 & \text{Dirac} \\ 2.00231930436(15) & \text{QED or Lamb-shift measurements} \end{cases}$$
We define the anomalous magnetic moment $a_e$ of the $e^-$: $g_e = 2(1 + a_e)$

Order by order expression:

\[
a_e (\text{QED}) = \frac{g_e - 2}{2} = \sum_{n=1}^{\infty} C_n \left( \frac{\alpha}{\pi} \right)^n
\]

Schwinger 1948: $C_1 = \frac{1}{2}$

Petermann, Sommerfield 1957: + all $\alpha^2$, e.g.

\[
C_2 = \frac{197}{14} + 12 \pi^2 - \frac{1}{2} \pi^2 \ln 2 + \frac{3}{4} \sum_{i=1}^{\infty} n^{-3} = -0.28478965579 \equivalent{\Rightarrow}
\]

S. Laporta et al. 1993: $C_3 = 1.181241456 \equiv$

2007 value containing over 100 Feynman diagrams:

\[
a_e = a_e (\text{QED}) \left\{ +a_e (\mu) + a_e (\tau) + a_e (\text{hadron}) + a_e (\text{weak}) \right\} = 1 159 652 180.85(.76) \times 10^{-12}
\]

\[ a_e(\text{QED}) = \frac{g_e - 2}{2} = C_1 \left( \frac{\alpha}{\pi} \right) + C_2 \left( \frac{\alpha}{\pi} \right)^2 + C_3 \left( \frac{\alpha}{\pi} \right)^3 + C_4 \left( \frac{\alpha}{\pi} \right)^4 + \ldots \]

Antihydrogen experiment Athena in CERN

Fundamental question: Are $g_e$ and $g_{e^+}$ identical?

Penning-trap with silicon detectors


<table>
<thead>
<tr>
<th>$K^0$</th>
<th>$\bar{K}^0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>relative mass difference</td>
<td>relative accuracy</td>
</tr>
<tr>
<td>charge/mass ($q/m$)</td>
<td>magnetic moment ($g-2$)</td>
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</table>

Relative mass difference

Upper limits
Parity Violation in Atoms (Weak Interaction)

\[ \Psi_{s_{1/2}}^{GSW} = \Psi_{s_{1/2}} + \epsilon \Psi_{p_{1/2}} \]

induces an E1 transition violation of Laporte selection rule

\[ H_{PV} = \frac{G_F}{2\sqrt{2}} \sum_{i,M} Q_{W,M} \gamma_i^5 \rho_M(\vec{r}_M) + \frac{G_F}{\sqrt{2}} \sum_{i,N} \left( f_{NC} + f_{HF} + f_A \right) \bar{\alpha}_i \bar{I}_M \rho_M(\vec{r}_M) + \ldots \]

\[ G_F = 1.16637 \times 10^{-11} \text{ MeV}^{-2} = 2.22255 \times 10^{-14} \text{ a.u.} \]

Experiments:

Bi Novosibirsk 1978 (876 nm)
Moscow, Oxford

Tl 6\text{P}_{1/2} - 7\text{P}_{1/2} Berkeley 1979
Seattle

Pb Seattle

Cs 6\text{S}_{1/2} - 7\text{S}_{1/2} Paris, Boulder 1997

Accuracy of 0.35 % in PNC

Fr 7\text{S}_{1/2} - 8\text{S}_{1/2} Stony Brook

Ba\text{+} Washington

Dy Berkeley

Conclusion: Theory and experiments agree, Standard model works
Gravitational fields do not enter into the SM (quantum gravitation, gravitons).

Thermodynamics does not enter directly into the SM (quantum thermodynamics, nonlinear QM, forward time direction): http://www.quantumthermodynamics.org/

Dark Matter and Dark Energy (if it exists) is currently assumed to explain the inflation of our universe (structure and galaxy formation, anisotropies in cosmic microwave background, new state of matter?).

The Particle/Antiparticle imbalance in our universe (10,000:1) cannot be explained by the SM (CPT violation and conservation of baryon number violation. NB: CPT violation implies loss of Lorentz-invariance)

Limitation of 3 lepton and quark families cannot be explained by the SM (new particles?)

Hierarchy problem of the SM (why is the gravitational force so much weaker than any other force, ie. $10^{32}$ times weaker than the weak force)

Values for Particle masses and fundamental constants only enter the SM as predetermined (fixed) entities (Higgs mechanism, variation of masses and fundamental constants in space-time, neutrino masses)

Electron EDM assumed to be too small from SM prediction
The exception tests the rule. Or, put another way, **The exception proves that the rule is wrong.** That is the principle of science. If there is an exception to any rule, and if it can be proved by observation, that rule is wrong.  

*Richard Feynman*

---

**Find breakdown of the standard model:**
- Variation of fundamental constants in space-time
- Measurement of electron dipole moment
- Deviations from atomic PV measurements
- Search for breakdown of CPT symmetry
- Search for the Higgs boson and new particles

---

**Extend the SM / develop new theory:**
- String Theory, M-theory, SUSY, Kaluza-Klein, …
I GUESS EVERYONE HAS A DIFFERENT VISION FOR THE PERFECT WORLD
Large Numbers hypothesis: Very large (or small) dimensionless universal constants cannot be pure mathematical numbers and must not occur in the basic laws of physics. (P.A.M. Dirac, 1937)
It is a fact that for the electron pure numbers appear, which have a magnitude completely different to 1; the ratio of the electron radius to the world radius of its mass, which is of a magnitude of $10^{40}$. 
Dirac’s large number hypothesis concerns the large ratio of the electric vs. the gravitational force between two electrons, which is \( \sim 10^{40} \); there is no rationalization of why such a huge number should appear in any physical theory. (Anything in-between?)

The SM contains \( 21(+x) \) fundamental constants, plus we need to add the gravitational constant outside the SM.

Some of these constants are intrinsically connected to certain theories.

These constants can not be obtained from the SM or its extensions.

There are “indications” that these constants may have changed over time and are connected to the big-bang event.

If the fine structure constant (velocity of light \( c \)) changes over time relativistic effects become observable!
The fundamental constants intrinsic to theory
The fundamental constants - Metrology

- The 22(+x) fundamental constants:
  - Masses (14): the mass of the up quark, down quark, charmed quark, strange quark, top quark, bottom quark, electron, (electron neutrino), muon, μ-neutrino, tauon, τ-neutrino, W, Z, Higgs
  - Coupling constants (4): the \( \alpha_{\text{EM}} \) coupling constant, \( \alpha_s \) strong coupling constant, \( \alpha_s \) SU(2) coupling constant, \( \alpha_s \) SU(3) strong coupling constant, cosmological constant \( G \)
    
    \[
    \begin{align*}
    c &= 299,792,458 \text{ m/s}, \\
    \hbar &= 4.054,571,596(82) \times 10^{-34} \text{ J s}, \\
    G &= 6.674(10) \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}, \\
    m_e &= 9.109,381,88(72) \times 10^{-31} \text{ kg}, \\
    e &= 1.602,176,462(63) \times 10^{-19} \text{ C}.
    \end{align*}
    \]

- Cabibbo-Kobayashi-Maskawa matrix (4): quark oscillations
- Pontecorvo-Maki-Nakagawa-Sakata matrix (4): neutrino oscillations
Any study on the variation of constants is linked to the definition of the system of units and to the theory of measurement. The choice of base units affects the possible time variation of constants.

**Solution:** Focus on dimensionless fundamental constants.

Our group focuses on the variation of the electron/proton ratio $\mu = m_e/m_p$ and the fine-structure constant $\alpha_{EM} (\equiv \alpha)$ in molecular spectra.

Antropic principle: The fine-tuning of the fundamental constants is required for life to exist. Slightly different coupling constants for the low-energy resonance in the production of carbon from helium in stars, $^{3}\text{He}\rightarrow^{12}\text{C}$ (CNO cycle), results in no resonance and therefore no life.

If $\alpha_S$ varies by 0.5% and $\alpha_{EM}$ by 4%, the stellar production of carbon or oxygen will be reduced by a factor 30–1000.


The variation of coupling constants in space provides a natural explanation of this fine tuning: we appear in an area of the universe where values of fundamental constants are suitable for our existence.
Roger Penrose (1989): "The argument can be used to explain why the conditions happen to be just right for the existence of (intelligent) life on the earth at the present time. For if they were not just right, then we should not have found ourselves to be here now, but somewhere else, at some other appropriate time."

Weak anthropic principle (WAP) (Brendon Carter): “We must be prepared to take account of the fact that our location (in time and space) in the universe is necessarily privileged to the extent of being compatible with our existence as observers.”

Strong anthropic principle (SAP) (Brendon Carter): “The Universe (and hence the fundamental constants on which it depends) must be such as to admit the creation of observers within it at some stage.”
Variation of fundamental constants (FC)

Change in property due to change in fundamental constants:

\[ P(\alpha, \mu, \cdots) = P(\alpha_0, \mu_0, \cdots) + \left( \frac{\partial P}{\partial \alpha} \bigg|_0 \right) \Delta \alpha + \left( \frac{\partial P}{\partial \mu} \bigg|_0 \right) \Delta \mu + \left( \frac{\partial P}{\partial g_n} \bigg|_0 \right) \Delta g_n + \cdots \]

If fundamental constants change, the frequency of any atomic or molecular transition also changes:

\[ \omega = \omega_0 \left[ 1 + Q_{\alpha} \frac{\delta \alpha}{\alpha} + Q_{\mu} \frac{\delta \mu}{\mu} + Q_{g_n} \frac{\delta g_n}{g_n} + \cdots \right] \]

In order to detect this variation we need to compare at least two transition frequencies (reference clock):

\[ \frac{\omega_i}{\omega_k} = \left( \frac{\omega_i}{\omega_k} \right)_0 \left[ 1 + \frac{\Delta \phi}{\phi} \right], \quad \phi = \alpha^{Q_{\alpha}} \mu^{Q_{\mu}} g_n^{Q_{g_n}} \]

Clearly, the effect is proportional to the differences in the sensitivity coefficients \( Q_{\lambda} \).
For optical transitions in light ($Z < 30$) atoms and molecules $Q_\alpha Q_\mu Q_g \ll 1$.

For optical transitions in heavy ($Z \geq 80$) atoms and molecules $Q_\alpha \approx 1$.

- Fine structure (IR, FIR) $\sim \alpha^2$ $Q_\alpha = 2$.
- Vibrational structure (IR) $\sim \mu^{1/2}$ $Q_\mu = 1/2$.
- Rotational structure (FIR, microwave) $Q_\mu = 1$.
- Magnetic hyperfine structure (microwave) $Q_\alpha = 2$; $Q_\mu = 1$; $Q_g = 1$.
- Tunneling transitions in polyatomic molecules (FIR, microwave) $1 \leq Q_\mu \leq 10$ (from WKB approximation).
- Microwave mixed tunneling-rotational lines $|Q_\mu| >> 1$.
- Microwave $\Lambda$-doublet lines in diatomics $|Q_\alpha|$, $|Q_\mu| >> 1$.

Courtesy: Mikhail Kozlov (Petersburg)
We can group the methods to measure spatial or temporal variation of FC into 3:

- **atomic and molecular methods**, including atomic clocks, quasar absorption and emission spectra (high-resolution spectroscopy), and observation of the cosmic microwave background (CMB) radiation (observables: spectra)

- **nuclear methods**, including nucleosynthesis, $\alpha$ and $\beta$ decay, Oklo reactor, quasar absorption spectra, big bang nucleosynthesis (observables: abundances, lifetimes, and cross sections)

- **gravitational methods**, including violation of the universality of free fall, stellar evolution, gravitational red-shift (Pound-Rebka experiment, Otago experiment, ….)

Experiments are either **lab-experiments** (duration ~ 1 yr, lifetime of a PhD student) or **field-experiments** (geochemical, astrophysical, and cosmological observations) of past events (duration < $10^{10}$ yr)
Time variation of a fundamental dimensionless constant

Robert J. Scherrer
Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235

We examine the time variation of a previously-uninvestigated fundamental dimensionless constant. Constraints are placed on this time variation using historical measurements. A model is presented for the time variation, and it is shown to lead to an accelerated expansion for the universe. Directions for future research are discussed.

PACS numbers: 98.80.Cq

It is well-known that only time variation of dimensionless fundamental constants has any physical meaning. Here we consider the time variation of a dimensionless constant not previously discussed in the literature: $\pi$. It is impossible to overstate the significance of this constant. Indeed, nearly every paper in astrophysics makes use of it. (For a randomly-selected collection of such papers, see Refs. [2, 3, 4, 5, 6, 7, 8, 9, 10]).

<table>
<thead>
<tr>
<th>Location</th>
<th>Time</th>
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<td>1900 BC</td>
<td>3.125</td>
</tr>
<tr>
<td>India</td>
<td>900 BC</td>
<td>3.139</td>
</tr>
<tr>
<td>China</td>
<td>263 AD</td>
<td>3.14</td>
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<tr>
<td>China</td>
<td>500 AD</td>
<td>3.1415926</td>
</tr>
<tr>
<td>India</td>
<td>1400 AD</td>
<td>3.14159265359</td>
</tr>
</tbody>
</table>


Past Event Measurements

- Afterglow Light Pattern 400,000 yrs.
- Dark Ages
- Development of Galaxies, Planets, etc.
- Dark Energy Accelerated Expansion
- Inflation
- Quantum Fluctuations
- Wilkinson Microwave Anisotropy Probe

**Big Bang**

- 10^{-12} s first elementary particles
- 4 min \(^1\text{H}^+\), \(^2\text{H}^+\), \(^4\text{He}^{2+}\)
- 300,000 years first atoms
- 1st Stars about 400 million yrs.

**Past Event Measurements**

- 13.7 billion years Big Bang Expansion
- formation of molecules in planetesimals (small bodies, precursors of planets) and dust grains
- synthesis of heavier elements in the interior of stars
In 1972, French uranium mining engineers discovered several zones of depleted uranium (0.44 % 235-U, 99.2745 % 238-U) near the Oklo River in Gabon. They concluded that this region was once a natural nuclear reactor part of a much larger one of the earth's continental crust. This contradicts typical 235-U abundance on earth (~0.72%).

Andrew Karam (2005): $2 \times 10^9$ years ago 235-U was present at 3.68 % abundance and a natural nuclear reactor achieving critical mass.

The ratio of the two light isotopes of samarium 149-Sm/147-Sm (which are not fission products) is ~0.9 on earth, but 0.02 in Oklo ores.

This comes from the neutron capture $n + ^{149}_{62}$Sm $\rightarrow ^{150}_{62}$Sm + $\gamma$ from which (neutron cross section) we can determine a limit for the $\alpha_{EM}$ variation in time (also sensitive to $m_q/\alpha_{QCD}$)

$$|\dot{\alpha}_{EM}/\alpha_{EM}| < 10^{-17} \text{ yr}^{-1}$$

Observation of distant astrophysical objects. I. Atoms
Quasar (QSO) absorption spectra:

\[ \Delta t = 10^{10} \text{ yr} \]

\[
\frac{\delta \nu}{\nu} \frac{\Delta t}{Q_\mu} = Q_\mu \frac{\dot{\mu}}{\mu} + Q_\alpha \frac{\dot{\alpha}}{\alpha}
\]

More recently: Murphy et al 2007 for the fine-structure constant (QSO):

\[ \Delta \alpha_{\text{EM}} / \alpha_{\text{EM}} = (20.96 \pm 0.17) \times 10^{-5} \]

\[ \Delta \alpha_{\text{EM}} / \alpha_{\text{EM}} = (-0.64 \pm 0.36) \times 10^{-5} \]

\[ |\dot{\alpha}_{\text{EM}} / \alpha_{\text{EM}}| < 8 \times 10^{-17} \text{ yr}^{-1} \]
Evidence for spatial variation of the fine structure constant

J. K. Webb\textsuperscript{1}, J. A. King\textsuperscript{1}, M. T. Murphy\textsuperscript{2}, V. V. Flambaum\textsuperscript{1}, R. F. Carswell\textsuperscript{3}, and M. B. Bainbridge\textsuperscript{1}

\textsuperscript{1}School of Physics, University of New South Wales, Sydney, NSW 2052, Australia
\textsuperscript{2}Centre for Astrophysics and Supercomputing, Swinburne University of Technology, Mail H39, PO Box 218, Victoria 3122, Australia and
\textsuperscript{3}Institute of Astronomy, Madingley Road, Cambridge, CB3 0HA, England.


We previously reported observations of quasar spectra from the Keck telescope suggesting a smaller value of the fine structure constant, $\alpha$, at high redshift. A new sample of 153 measurements from the ESO Very Large Telescope (VLT), probing a different direction in the universe, also depends on redshift, but in the opposite sense, that is, $\alpha$ appears on average to be larger in the past. The combined dataset is well represented by a spatial dipole, significant at the 4.1$\sigma$ level, in the direction right ascension $17.3 \pm 0.6$ hours, declination $-61 \pm 9$ degrees. A detailed analysis for systematics, using observations duplicated at both telescopes, reveals none which are likely to emulate this result.

\begin{equation}
\Delta \alpha / \alpha = \left(1.1 \pm 0.2\right) \times 10^{-6} \text{ GLyr}^{-1} r \cos \theta + \left(-1.9 \pm 0.8\right) \times 10^{-6}
\end{equation}
Laws of Physics Vary Throughout the Universe, New Study Suggests

ScienceDaily (Sep. 9, 2010) — A team of astrophysicists based in Australia and England has uncovered evidence that the laws of physics are different in different parts of the universe.

The team -- from the University of New South Wales, Swinburne University of Technology and the University of Cambridge -- has submitted a report of the discovery for publication in the journal Physical Review Letters. A preliminary version of the paper is currently under peer review.

The report describes how one of the supposed fundamental constants of Nature appears not to be constant after all. Instead, this 'magic number' known as the fine-structure constant -- 'alpha' for short -- appears to vary throughout the universe.

"After measuring alpha in around 300 distant galaxies, a consistency emerged: this magic number, which tells us the strength of electromagnetism, is not the same everywhere as it is here on Earth, and seems to vary continuously along a preferred axis through the universe," Professor John Webb from the University of New South Wales said.
Potential systematic errors

- Laboratory wavelength errors
- Data quality variations
- Heliocentric velocity variation
- Isotopic ratio shifts
- Hyperfine structure shifts
- Magnetic fields
- Wavelength miscalibrations
- Temperature changes during observation
- Line blending
- Atmospheric refraction effects
- Instrumental profile variation

Michael Murphy, UNSW
Observation of distant astrophysical objects - Molecules

2 atoms (34): H₂, AlF, AlCl, C₂, CH, CH⁺, CN, CO, CO⁺, CP, CS, CSi, HCl, KCl, NH, NO, NS, NaCl, OH, PN, SO, SO⁺, SiN, SiO, SiS, …

3 atoms (31): H₃⁺, C₃, C₂H, C₂O, C₂S, CH₂, HCN, HCO, HCO⁺, HCS⁺, HOC⁺, H₂O, H₂S, HNC, HNO, MgCN, MgNC, N₂H⁺, N₂O, NaCN, OCS, SO₂, c-SiC₂, CO₂, NH₂, …

4 atoms (22): c-C₃H, l-C₃H, C₃N, C₃O, C₃S, C₃H₂, CH₂D⁺?, HCCN, HCNH⁺, HNCO, HNCS, HOCO⁺, H₂CO, H₂CN, H₂CS, H₃O⁺, NH₃, SiC₃,…

5 atoms (18): C₅, C₄H, C₄Si, l-C₃H₂, c-C₃H₂, CH₂CN, CH₄, HC₃N, HC₂NC, HCOOH, H₂CHN, H₂C₂O, H₂NCN, HNC₃, SiH₄, H₂COH⁺.

6 atoms (16): C₅H, C₅O, C₂H₄, CH₃CN, CH₃NC, CH₃OH, CH₃SH, HC₃NH⁺, HC₂CHO, HCONH₂, l-H₂C₄, C₅N, HC₄N, CH₂CNH.

7 atoms (9): C₆H, CH₂CHCN, CH₃C₂H, HC₄CN, HC₅N, HCOCH₃, NH₂CH₃, H₂CHCOH.

8 atoms (10): CH₃C₂CN, HOCH₂-CHO, HCOOCH₃, CH₃COOH, H₂C₆, C₇H, CH₃CONH₂,…

9 atoms (9) CH₃C₄H, (CH₃)₂O, CH₃CH₂CN, CH₃CONH₂, CH₃CH₂OH, HC₇N, C₈H, …

> 9 atoms (11): CH₃C₅N, (CH₃)₂CO, HC₉N, HC₁₁N, CH₃CH₂CHO, C₆₀, NH₂CH₂COOH ?,…

http://science.gsfc.nasa.gov/691/cosmicice/interstellar.html
The interstellar molecule $\text{NH}^+$ - Results from our lab

The interstellar molecule NH$^+$

Results from our lab: rotational spectrum

\[ E[\text{cm}^{-1}] \quad ^2\Pi_{1/2} \quad ^2\Pi_{3/2} \quad ^4\Sigma^- \]

<table>
<thead>
<tr>
<th>$N$</th>
<th>$J$</th>
<th>$v = 0$</th>
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<td>4</td>
<td>+ 9/2</td>
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<tr>
<td>9/2</td>
<td>3</td>
<td>+ 7/2</td>
</tr>
<tr>
<td>7/2</td>
<td>2</td>
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<td>+ 3/2</td>
</tr>
<tr>
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$\quad$ $\quad$ $\quad$

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<td>+ 5/2</td>
</tr>
<tr>
<td>1/2</td>
<td>2</td>
<td>+ 3/2</td>
</tr>
</tbody>
</table>

K. Beloy, M. G. Kozlov, A. Borschevsky, A. Hauser, V. V. Flambaum, P. Schwerdtfeger, 
Results for sensitivity factors

Low-frequency ($|\omega| < 30 \text{ cm}^{-1}$) transitions $^2\Pi \rightarrow ^4\Sigma^-$. Negative frequencies mean that the $^4\Sigma^-$ level is below the $^2\Pi$ level. $^4\Sigma^-$ levels are labeled with quantum numbers $N^p_J$ and $^2\Pi$ levels are labeled with $\Omega^p_J$. $E$ and $\omega$ are in cm$^{-1}$ and $||E1||^2$ is in atomic units. Transitions with $||E1||^2 < 10^{-3}$ a.u. are skipped.

\[
\frac{\delta \omega}{\omega} = Q_\mu \frac{\delta \mu}{\mu} + Q_\alpha \frac{\delta \alpha}{\alpha}
\]

| $N^p_J$ | $\Omega^p_J$ | $E_\Sigma$ | $\omega$ | $Q_\alpha$ | $Q_\mu$ | $||E1||^2$ |
|---------|--------------|-------------|----------|------------|----------|-------------|
| $2_{7/2}^-$ | $3/2^+_{9/2}$ | 443.287 | -24.658 | -3.74 | 17.82 | 0.005 |
| $4_{11/2}^-$ | $1/2^+_{13/2}$ | 643.977 | -0.983 | -76.84 | 249.78 | 0.002 |
| $4_{11/2}^-$ | $3/2^+_{11/2}$ | 643.977 | -7.866 | -4.68 | 30.10 | 0.165 |
| $4_{9/2}^-$ | $3/2^+_{11/2}$ | 649.676 | -2.167 | -48.45 | 193.99 | 0.001 |

Transitions for $v = 0$

| $0_{3/2}^-$ | $1/2^+_{1/2}$ | 0.000 | -6.976 | -13.68 | 22.48 | 0.385 |
| $1_{3/2}^+$ | $1/2^+_{1/2}$ | 21.486 | 5.055 | 19.73 | -33.94 | 0.208 |
| $1_{1/2}^+$ | $1/2^-_{3/2}$ | 58.529 | -5.931 | -19.95 | 25.71 | 0.222 |
| $2_{5/2}^-$ | $1/2^+_{3/2}$ | 77.352 | 12.474 | 3.48 | -8.68 | 0.023 |
| $2_{5/2}^-$ | $1/2^-_{3/2}$ | 83.854 | 18.976 | 5.44 | -6.48 | 0.003 |
| $2_{1/2}^-$ | $3/2^+_{3/2}$ | 104.966 | -29.795 | -0.10 | 5.94 | 0.099 |
| $3_{1/2}^+$ | $3/2^-_{5/2}$ | 190.451 | -26.037 | -1.96 | 7.87 | 0.003 |

Transitions for $v = 1$

Problem: NH$^+$ not discovered yet in interstellar space

Do Lab-exp.
Better accuracy and control of exp.

Problem: For NH$^+$ we need at least $\delta \omega = 10^{-4}$ Hz/yr
Electric field gradients required for nuclear quadrupole coupling in rotational spectra are extremely sensitive to relativistic effects:

- \( \Delta q \) [a.u.]
- \( \Delta_{\text{pic}} q(\text{Cl}) \)
- \( \Delta_{\text{pic}} q(\text{M}) \)
- \( \Delta_{\text{cor}} q(\text{Cl}) \)
- \( \Delta_{\text{cor}} q(\text{M}) \)
- \( \Delta_R q(\text{Cl}) \)
- \( \Delta_R q(\text{M}) \)

Nuclear quadrupole coupling in the rotational spectrum of interstellar KCl

\[
\Delta \text{EFG}_{\text{B3LYP}}^{\text{K}} = 4.4203 \times 10^{-5} \Delta \alpha - 1.0045 \times 10^{-6} \Delta \alpha^2
\]

\[
\Delta \text{EFG}_{\text{MP2}}^{\text{K}} = 5.8740 \times 10^{-5} \Delta \alpha - 1.1397 \times 10^{-6} \Delta \alpha^2
\]

\[
\Delta \text{EFG}_{\text{B3LYP}}^{\text{Cl}} = -1.6112 \times 10^{-4} \Delta \alpha - 1.1819 \times 10^{-6} \Delta \alpha^2
\]

\[
\Delta \text{EFG}_{\text{MP2}}^{\text{Cl}} = 1.0569 \times 10^{-4} \Delta \alpha - 1.1137 \times 10^{-7} \Delta \alpha^2
\]

\[
\Delta \text{NQCC}_{\text{MP2}}^{\text{K}} = 1.81 \times 10^{-12} \text{Hz/year}
\]

\[
\Delta \text{NQCC}_{\text{MP2}}^{\text{Cl}} = 4.44 \times 10^{-12} \text{Hz/year}
\]
Laboratory Experiments (Atomic Clocks) for time variation
Experiments linked to atomic clock for comparison

T. Rosenband et al., Science 319, 1808 (2008)

\[
\frac{\Delta \Omega}{\Omega} = \frac{\Delta \omega}{\omega} - \frac{\Delta \omega_{rc}}{\omega_{rc}}
\]

\[
27\text{Al} : \quad ^1S_0 \leftrightarrow ^3P_0
\]
\[
_{199}\text{Hg}^+: \quad ^2S_{1/2} \rightarrow ^2D_{5/2}
\]

\[F = 0 \rightarrow F = 2\]

electric quadrupole transition

In units of \(10^{-18}\) fractional frequency

<table>
<thead>
<tr>
<th>Shift</th>
<th>(\Delta \nu_{\text{Al}})</th>
<th>(\sigma_{\text{Al}})</th>
<th>(\Delta \nu_{\text{Hg}})</th>
<th>(\sigma_{\text{Hg}})</th>
<th>Limitation</th>
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<tbody>
<tr>
<td>Micromotion</td>
<td>-20</td>
<td>20</td>
<td>-4</td>
<td>4</td>
<td>Static electric fields</td>
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<tr>
<td>Secular motion</td>
<td>-16</td>
<td>8</td>
<td>-3</td>
<td>3</td>
<td>Doppler cooling</td>
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<tr>
<td>Blackbody radiation</td>
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<td>5</td>
<td>0</td>
<td>0</td>
<td>DC polarizability</td>
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<tr>
<td>313-nm Stark</td>
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<td>2</td>
<td>-</td>
<td>-</td>
<td>Polarizability, intensity</td>
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<td>DC quadratic Zeeman</td>
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<td>0.5</td>
<td>-1130</td>
<td>5</td>
<td>B-field calibration</td>
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<tr>
<td>AC quadratic Zeeman</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>10</td>
<td>Trap RF B-fields</td>
</tr>
<tr>
<td>Electric quadrupole</td>
<td>0</td>
<td>0.5</td>
<td>0</td>
<td>10</td>
<td>B-field orientation</td>
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<tr>
<td>First-order Doppler</td>
<td>0</td>
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<td>0</td>
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<td>Statistical imbalance</td>
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<tr>
<td>Background gas collisions</td>
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<td>1</td>
<td>-</td>
<td>-</td>
<td>Clock height</td>
</tr>
<tr>
<td>Total</td>
<td>-513</td>
<td>23</td>
<td>-1137</td>
<td>19</td>
<td></td>
</tr>
</tbody>
</table>

\[\alpha^1 \frac{d \alpha}{dt} = (-1.6 \pm 2.3) \times 10^{-17} / \]
Temporal variation of the SF$_6$ two-photon transition frequency
Comparison to Cs atomic clock

Chardonnet's new experiment in Paris

Data from 10 November 2004 to 28 June 2006

Frequency drift:
1.2 mHz/day (± 0.35 mHz)
i.e. $1.5 \times 10^{-14}$ kJ/mol/year

$\mu^1 d\mu/dt = (1.2 \pm 2.2) \times 10^{-16}$ yr$^{-1}$
Calculations for the $X^1\Sigma_g^+$ and $a^3\Sigma_u^+$ states
Program Dirac, Fock-space coupled
cluster calculations, vibrations by WKB

Long-range dominated by
relativistically reduced dipole polarizability

short-range dominated by
relativistically increased bond stability
Relativistic Electronic Structure Theory

A series of approximations: Towards the exact solution

\[ \hat{H}_D = \sum h_D^+ (i) + \sum g_{CB}^+ (i, j) + \hat{H}_{QED} + \Xi \]
\[
\begin{pmatrix}
V - E & c\vec{\sigma} \vec{P} \\
c\vec{\sigma} \vec{P} & -2mc^2 + V - E
\end{pmatrix}
\begin{pmatrix}
\varphi_L \\
\varphi_S
\end{pmatrix} = 0
\]
Problem: $H_D$ is unbound and the small component $\varphi_S$ of the Dirac bi-spinor only accounts for less than 1% of the total wavefunction. The unitary transformation from the Dirac- to the Schrödinger picture ($H_{tr}$ semi-bound):

\[
\begin{pmatrix}
V - E & c\vec{\sigma}\vec{p} \\
c\vec{\sigma}\vec{p} & -2mc^2 + V - E
\end{pmatrix}
\begin{pmatrix}
\varphi_L \\
\varphi_S
\end{pmatrix} = 0
\]

\[
H_{tr} = UH_DU^\dagger = \begin{pmatrix}
H_+ & 0 \\
0 & H_-
\end{pmatrix}
\]

\[
U = \begin{pmatrix}
(1 + X^\dagger X)^{-1/2} & (1 + X^\dagger X)^{-1/2} X^\dagger \\
-e^{i\varphi}(1 + X^\dagger X)^{-1/2} X & e^{i\varphi}(1 + X^\dagger X)^{-1/2}
\end{pmatrix}
\]

\[
X = \left(2mc^2 + E - V\right)^{-1} c\vec{\sigma}\vec{p}
\]

$\varphi_S = X\varphi_L, \quad \Phi = U\varphi_L, \quad (\Phi, \Phi) = 1$

X2C-approximation used for Cs$_2$

The Breit Pauli Operator

\[
H^{BP}_{s} = H_{NR} + H_{Breit-Pauli} = H_{NR} - \sum_{i} \frac{1}{8c^2} \tilde{p}_i^4 - \sum_{i} \frac{1}{4c^2} \tilde{\sigma}_i (\nabla V(\vec{r}_i) \times \vec{p}_i) - \sum_{i} \frac{1}{8c^2} \Delta V(\vec{r}_i)
\]

- mass-velocity
- spin-orbit
- Darwin

\[
- \sum \frac{1}{c^2 r_y^3} \tilde{\sigma}_i ((\vec{r}_j - \vec{r}_i) \times \vec{p}_j) - \sum \frac{1}{2c^2 r_{ij}^3} \tilde{\sigma}_i ((\vec{r}_i - \vec{r}_j) \times \vec{p}_i) - \sum \frac{\pi}{c^2} \delta(\vec{r}_i - \vec{r}_j)
\]

- spin-other orbit
- spin-orbit (2)
- Darwin (2)

\[
- \sum \frac{1}{2c^2} \tilde{p}_i \left[ \frac{(\vec{r}_i - \vec{r}_j)(\vec{r}_i - \vec{r}_j)}{r_{ij}^3} + \frac{1}{r_{ij}} \right] \tilde{p}_j - \sum \frac{1}{4c^2} \tilde{\sigma}_i \left[ \frac{3(\vec{r}_i - \vec{r}_j)(\vec{r}_i - \vec{r}_j)}{r_{ij}^5} - \frac{1}{r_{ij}^3} \right] \tilde{\sigma}_j - \sum \frac{2\pi}{3c^2} \delta(\vec{r}_i - \vec{r}_j) \tilde{\sigma}_i \tilde{\sigma}_j
\]

- orbit-other orbit
- spin-other spin
- spin-other spin (2)

**Advantage:** Useful for interpretation purposes (historical reasons)

**Disadvantage:** Unbound, essentially singular

Relativistic effects scale like \( \alpha^2 \), but linear scaling for temporal or spatial variation
\[
(\alpha_0 + \delta\alpha)^2 = 2\alpha_0 \delta\alpha + ...
\]
**Cs₂ – Sensitivity factors from WKB theory**

### Aim: Find 2 potential curves with very different $q_\alpha$ and $q_\mu$ behavior

\[
\delta \omega = q_\mu \frac{\delta \mu}{\mu} + q_\alpha \frac{\delta \alpha}{\alpha}
\]

Near degeneracy of vibration states of the two potential curves.

### Reduced sensitivity factors for excited states as antibonding orbital reduces relativistic effects

<table>
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<tr>
<th></th>
<th>$X^1\Sigma_g^+$</th>
<th>$a^3\Sigma_u^+$</th>
<th>$\Delta$</th>
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<tbody>
<tr>
<td>$q_\mu$ [cm$^{-1}$]</td>
<td>827</td>
<td>0</td>
<td>827</td>
</tr>
<tr>
<td>$q_\alpha$ [cm$^{-1}$]</td>
<td>-229</td>
<td>47</td>
<td>-276</td>
</tr>
<tr>
<td>$\rho$ [1/cm$^{-1}$]</td>
<td>0.065</td>
<td>0.086</td>
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</table>

Evaluated at $E = -279$ cm$^{-1}$

<table>
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<tr>
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<th>$a^3\Sigma_u^+$</th>
<th>$\Delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$q_\mu$ [cm$^{-1}$]</td>
<td>203</td>
<td>48</td>
<td>155</td>
</tr>
<tr>
<td>$q_\alpha$ [cm$^{-1}$]</td>
<td>-36</td>
<td>19</td>
<td>-55</td>
</tr>
<tr>
<td>$\rho$ [1/cm$^{-1}$]</td>
<td>0.34</td>
<td>0.39</td>
<td></td>
</tr>
</tbody>
</table>

Evaluated at $E = -17.4$ cm$^{-1}$

- **D: dissociation energy of Cs₂**

- **qµ (X\,Σ\,g\,\,+)**

- **qα (X\,Σ\,g\,\,+)**

- **qµ (a\,Σ\,u\,+)**

- **qα (a\,Σ\,u\,+)**

- **dissociation limit**

- **no upper states available**

- **Reduced sensitivity factors** for excited states as antibonding orbital reduces relativistic effects.
Te$_2$ - A potential candidate

Misha G. Kozlov (Petersburg)

David DeMille (Yale)
Back to NQC – Going for heavier elements

AuH

with $\dot{\alpha}/\alpha = -1.6 \times 10^{-17}$/year

$\Delta NQCC_{\text{B3LYP}} = -0.0207 \text{mHz}$

$\Delta NQCC_{\text{MP2}} = -0.0284 \text{mHz}$

$\Delta EFG_{\text{B3LYP}} = -0.07353 \Delta \alpha + 0.00095 \Delta \alpha^2$

$\Delta EFG_{\text{MP2}} = -0.10185 \Delta \alpha + 0.00120 \Delta \alpha^2$
Conclusions

- Best current limits are

\[ \alpha^{-1} \frac{d\alpha}{dt} = (-1.6 \pm 2.3) \times 10^{-17} \text{ yr}^{-1} \quad \text{(Rosenband et al., 2008)} \]
\[ \mu^{-1} \frac{d\mu}{dt} = (-1.2 \pm 2.2) \times 10^{-16} \text{ yr}^{-1} \quad \text{(Chardonnet et al., 2008)} \]
\[ G^{-1} \frac{dG}{dt} = (0 \pm 1.6) \times 10^{-16} \text{ yr}^{-1} \quad \text{(Guenther et al., 1998)} \]

- We need better candidates with enhanced sensitivity factors for properties which can be accurately determined by high-resolution spectroscopy. Large enhancements for quasi-degenerate narrow transitions according to V.V. Flambaum.

- Molecules currently considered are Cs\(_2\), CaH, MgH, CaH\(^+\), Cl\(_2\)\(^+\), IrC, HfF\(^+\), SiBr, LaS, LuO, NH\(_3\), H\(_3\)O\(^+\), CH\(_3\)OH, CH\(_3\)NH\(_2\), H\(_2\)O\(_2\),... Next molecules up: AuBr, Te\(_2\), ... In our group we so far considered SrBr, Hg\(_2\), Cs\(_2\) and NH\(^+\):

Thank You!

CTCP
Center for Theoretical Chemistry and Physics

L’art pour l’art, la science pour la science
The Theory of Everything for University Administrators
Beautiful theory collides with smashing particle data

Latest results from the LHC are casting doubt on the theory of supersymmetry.

By Geoff Brumfiel

"Wonderful, beautiful and unique" is how Gordon Kane describes supersymmetry theory. Kane, a theoretical physicist at the University of Michigan in Ann Arbor, has spent about 30 years working on supersymmetry, a theory that he and many others believe solves a host of problems with our understanding of the subatomic world.

Yet there is growing anxiety that the theory, however elegant it might be, is wrong. Data from the Large Hadron Collider (LHC), a 27-kilometer proton smasher that straddles the French-Swiss border near Geneva, Switzerland, have shown no sign of the "super particles" that the theory predicts. "We're painting supersymmetry into a corner," says Chris Lester, a particle physicist at the University of Cambridge, UK, who works with the LHC's ATLAS detector. Along with the LHC's Compact Muon Solenoid experiment, ATLAS has spent the past year hunting for super particles, and is now set to gather more data when the LHC begins a high-power run in the next few weeks. If the detectors fail to find any super particles by the end of the year, the theory could be in serious trouble.


Supersymmetry (known as SUSY and pronounced "Susie") emerged in the 1970s as a way to solve a major shortcoming of the standard model of particle physics, which describes the behavior of the fundamental particles that make up normal matter (see "The bestiary"). Researchers have now found every particle predicted by the model, save one: the Higgs boson, theorized to help endow other particles with mass.

The Higgs is crucial to the theory, but its predicted mass is subject to wild fluctuations caused by quantum effects from other fundamental particles. Those fluctuations can increase the Higgs' expected mass to a point at which other fundamental particles should be much more massive than they actually are, effectively breaking the standard model. Theorists can eliminate the fluctuations from their equations, but only by setting the Higgs mass to a very precise value—a fraction heavier or lighter and the whole theoretical edifice collapses. Many physicists are uncomfortable with any theory that requires such delicate fine-tuning to work.

SUSY offers an alternative to this "fine-tuning" problem. The theory postulates that each regular particle has a heavier supersymmetrical partner, many of which are unstable and rarely interact with normal matter. The quantum fluctuations of the supersymmetrical particles perfectly cancel out those of the regular particles, returning the Higgs boson to an acceptable mass range.

Theorists have also discovered that SUSY can solve other problems. Some of the lightest supersymmetrical particles could be the elusive dark matter that cosmologists have been hunting for since the 1950s. Although it has never been seen, dark matter makes up about 85 percent of the matter in the Universe, according to observations of how galaxies move.

SUSY can also be used to bring together all the forces except gravity into a single force at high energies, a big step towards a "theory of everything" that unifies and explains all known physics—one of the ultimate goals of science. Perhaps most important for some theorists, "SUSY is very beautiful mathematically," says Ben Allanach, a theorist at the University of Cambridge.

SUSY's utility and mathematical grace have instilled a "religious devotion" among its followers, says Adam Falkowski, a theorist at the University of Paris-South in France. But colliders have failed to turn up direct evidence of the super particles predicted by the theory. The Tevatron at the Fermi National Accelerator Laboratory in Batavia, Illinois, for example, has found no evidence of supersymmetrical quarks ("squarks") at masses of up to 379 gigaelectronvolts (energy and mass are used interchangeably in the world of particle physics).

The LHC is now rapidly accumulating data at higher energies, ruling out heavier territory for the super particles. This creates a serious