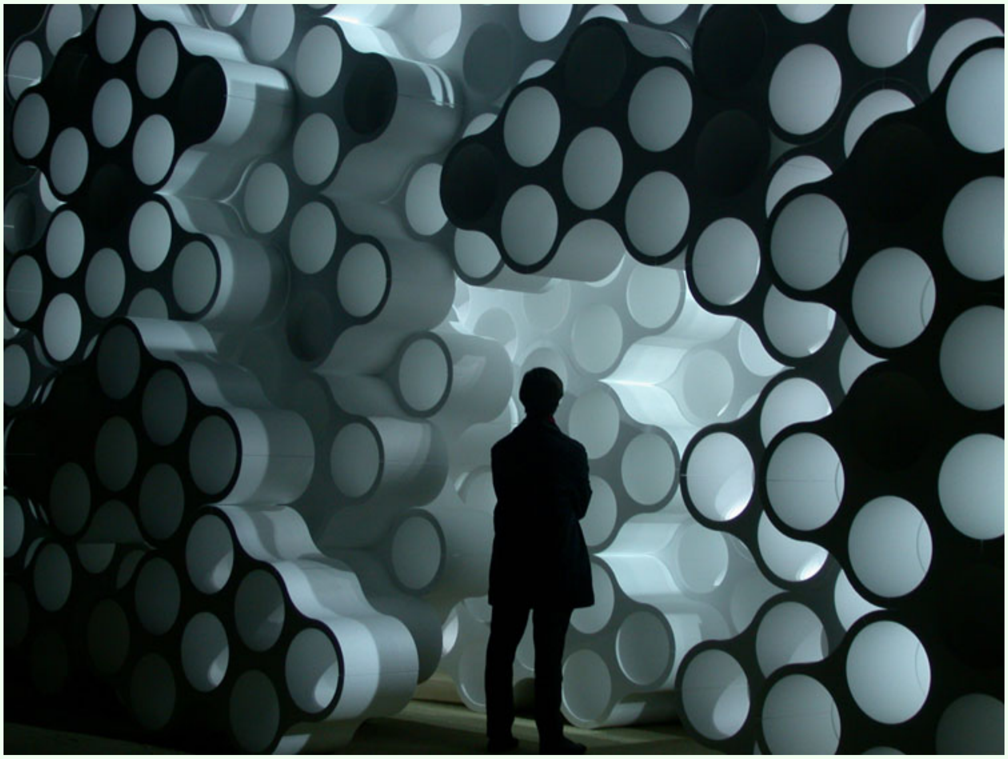
INSIDE THE HYDROGEN ATOM

Marek Nowakowski
Departamento de Fisica, Universidad de los Andes



Collaborators: N. G. Kelkar
D. Bedoya Fierro and A. Bermudez Manjarres

1 Motivation

Why bother? After all Hydrogen atom is the oldest bound states in quantum mechanics

2 Scalar forces in the hydrogen atom

Beyond

$$\frac{1}{r}$$

$\longrightarrow$ finite size of the proton

$\longrightarrow$ Breit equation and the two Darwin terms

3 The role of $\gamma\gamma$ corrections

Electric potentials in the Euler-Heisenberg theory

perturbative and non-perturbative solutions

application on the electric proton potential

4 Consequences for the energy levels

Calculating the energy correction $\Delta\mathcal{E}$

5 Outlook

From hydrogen atom to heavier elements

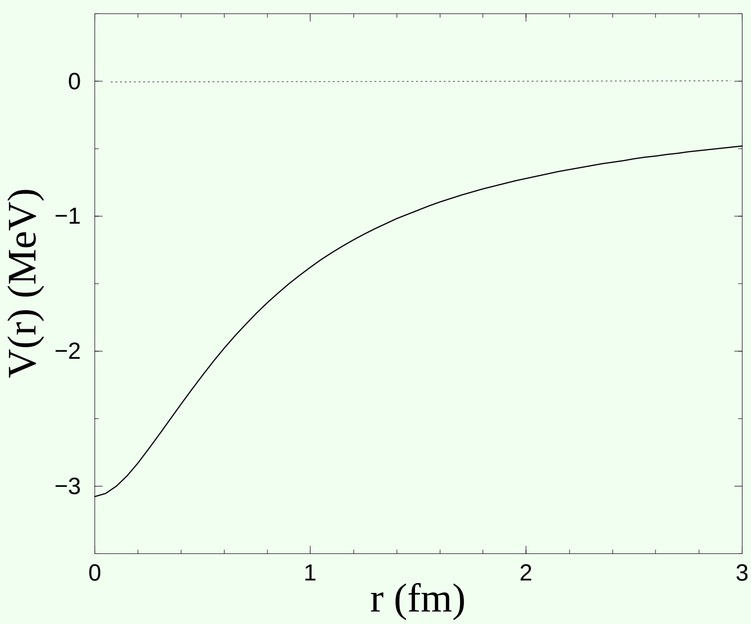
Niels Bohr: "A physicist is just an atom's way of looking at itself"

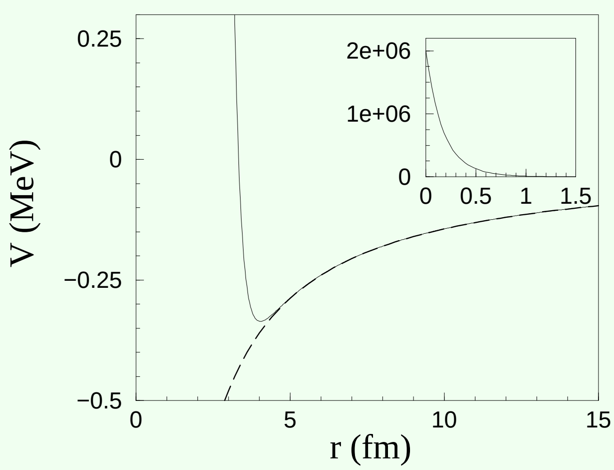
$$\hbar = c = k_B = 1$$

But not always

1. Motivation

Have an unbiased look at the following (interaction) potentials

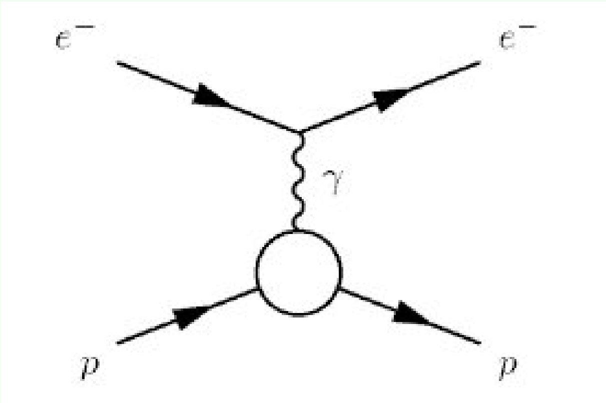




The first one resembles the Wood-Saxon potential with depth of -3 MeV. The second one has minimum at -0.3 MeV , but also a repulsive core with a height of 2×10^3 MeV . Nuclear potentials? A variational principle reveals that the ground state is close to -13 eV Indeed, the potentials reflect the Finite Size of the proton.

2. Scalar forced in the Hydrogen atom

Formalism: potentials from QFT
scattering amplitude $\sim$ FourierTransform[potential]
Breit equation $\sim$ InverseFourierTransform[elastic e-p amplitude]



vertex with two electromagnetic form-factors:

$$e\gamma_\mu \to e\left(F_1(q^2)\gamma_\mu + \frac{F_2(q^2)}{2m_p}\sigma_{\mu\nu}q^\nu\right)$$

Sachs form-factors:

$$G_E = F_1 + \frac{q^2}{4m_p} F_2$$

$$G_M = F_1 + F_2$$

The Breit Hamiltonian (H. A. Bethe and E. E. Salpeter "Quantum Mechanics of one- and two-electron atoms"):

$$V_{ep}(\boldsymbol{q}) = e\left[\frac{G_E(\boldsymbol{q})}{\boldsymbol{q}^2} - \frac{1}{8m_p^2} G_E(\boldsymbol{q}) - \frac{1}{8m_e^2} G_E(\boldsymbol{q})\right]$$

$$+F(\boldsymbol{\sigma}_e, \boldsymbol{\sigma}_p; \boldsymbol{p}_p, \boldsymbol{p}_e)$$

$$= \text{(modified) Coulomb} + \text{Proton Darwin}$$

$$+ \text{ electron Darwin}$$

$$= eV_p(\boldsymbol{q}) + V_{eD}(\boldsymbol{q})$$

where V_p is the electric potential of the proton in momentum space.

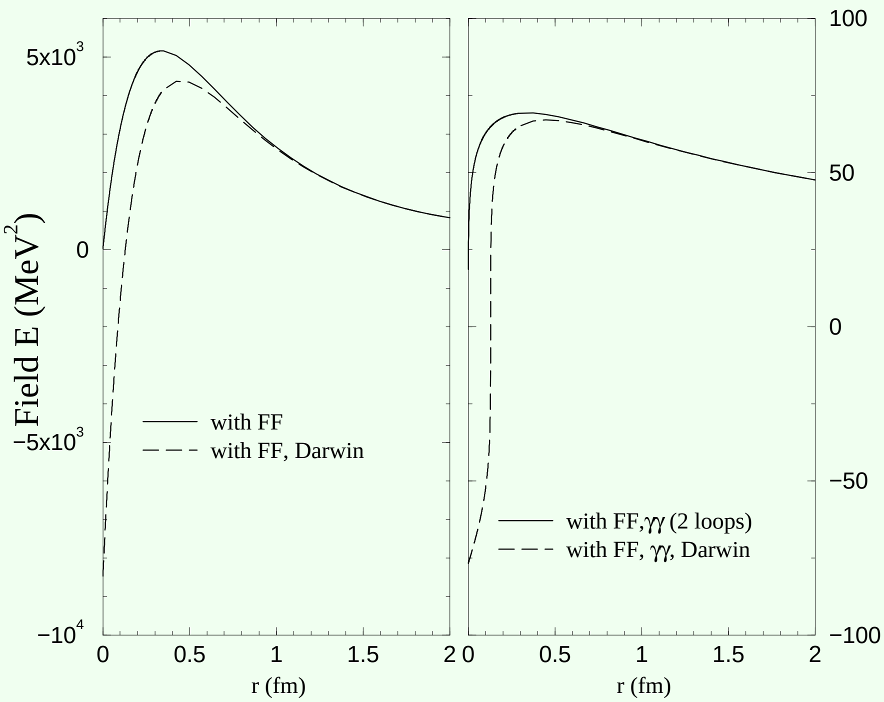
$$V_{ep}(\boldsymbol{r}) = \int \frac{d^3q}{(2\pi)^3} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} V_{ep}(\boldsymbol{q})$$

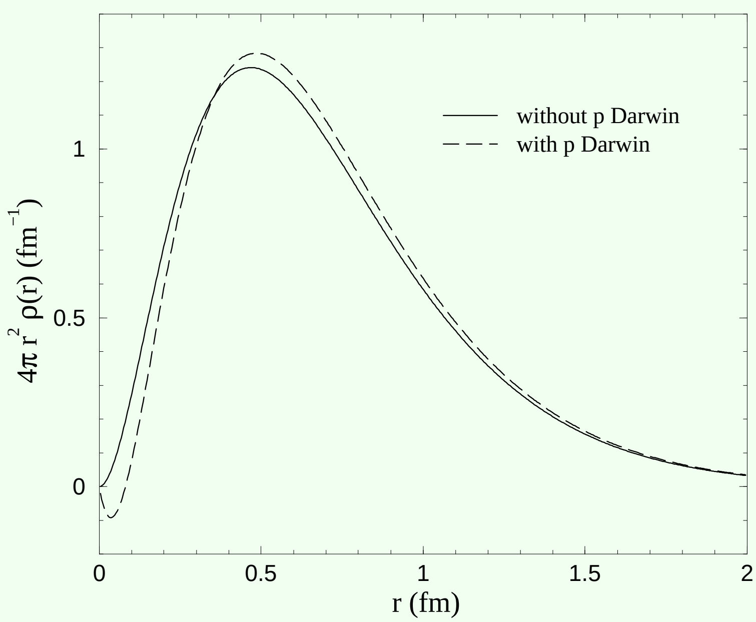
$$= eV_C(\boldsymbol{r}) + V_{pD}(\boldsymbol{r}) + V_{eD}(\boldsymbol{r}) = eV_p(\boldsymbol{r}) + V_{eD}(\boldsymbol{r})$$

Obviously, we have

$$V_{eD}(\boldsymbol{r}) \propto V_{pD}(\boldsymbol{r}) \propto \rho(\boldsymbol{r}) \propto \int dq^3 e^{i\boldsymbol{q}\cdot\boldsymbol{r}} G_E(\boldsymbol{q})$$

We have identified the electric potential of the proton from the Breit equation as terms which are (i) scalar (no spin and no momentum terms and (ii) independent form the properties of the test particle. By this token the proton Darwin term is part of the electric potential, but the electron Darwin not. This has some consequences for the electric field at small distances inside the proton and also for the charge distribution.


Field E (MeV^2)
$5x10^3$
0
$-5x10^3$
-10^4
0
0.5
1
1.5
2
r (fm)
with FF
with FF, Darwin
100
50
0
−50
−100
with FF,γγ (2 loops)
with FF, γγ, Darwin

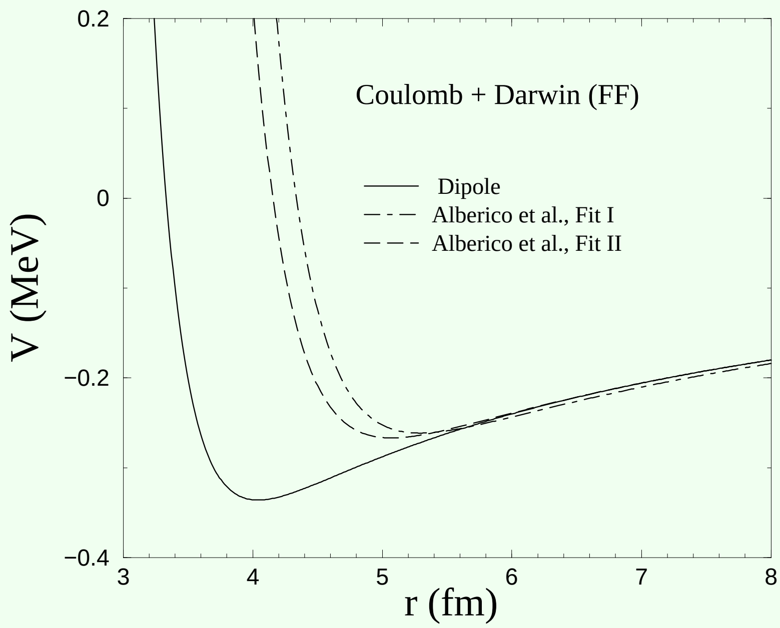


Via $\boldsymbol{\nabla} \cdot \boldsymbol{E} = \frac{2}{r}E + \frac{dE}{dr} \propto \rho$ the charge distribution is non-zero at the center when we include the proton Darwin term in the potential. With the dipole parametrization $G_E(\boldsymbol{q}^2) = 1/(1+\boldsymbol{q}^2/m^2)^2$, one can obtain analytical formulae, e.g.,

$$V_p(r) = V_p^C + V_p^{pD}$$

$$V_p^C = \frac{e}{r}\left(1 - e^{-mr}\left(1 + \frac{er}{2}\right)\right)$$

But the main issues (of this talk) will remain mostly insensitive to the parametrization of the electric form-factors.



One does not see nowadays these results very often since the simplest estimate of the correction to the energy level(s) of the hydrogen atom is

$$\Delta\mathcal{E} = \int d^3x |\Psi(x)|^2 \left[eV_p(r) + \frac{Ze^2}{r} \right]$$

$$\simeq |\Psi(0)|^2 \int d^3x \left[eV_p(r) + \frac{Ze^2}{r} \right]$$

which after integration by parts becomes

$$\frac{e}{6} |\Psi(0)|^2 \int d^3x r^2 \nabla^2 V_p$$

Using the Poisson equation the definition of the radius as the second moment of the charge distribution

$$< r^2 > = \int d^3x \rho r^2$$

one gets finally

$$\Delta\mathcal{E} = \frac{e}{6} |\Psi(0)|^2 Ze < r^2 >$$

Seemingly one does not need to know anything about the electric fields inside the proton as everything is encoded in the proton radius. However, some obvious questions cross the mind.

- Are these fields really so strong?
- Is there a danger of pairs production? Indeed, one can calculate the energy content in the electric field

$$\int d^3xE^2 \propto \mathscr{E}(field) \simeq 1 \ MeV$$

  which is very close to $2m_e$ and given the uncertainty of the form-factors at the border to the pair production threshold.
- By $e \rightarrow -e$ one obtains the positron proton potential with a potential depth of 10^6 MeV!

Below I will discuss the possibility how $\gamma\gamma$ contribution lower the electric field strength well below the pair production threshold, but at the price that the simple and useful relation $\Delta\mathcal{E} \propto < r^2 >$ cannot be maintained anymore. Before going into the details let me recall some special quantum mechanical aspects of the Finite Size contribution of the proton.

- The field/potential of the proton at small r is large but still finite as compared to $1/r$. Therefore, it is not a correction, but its short range allows us to treat in as a correction in $\Delta\mathcal{E}$.

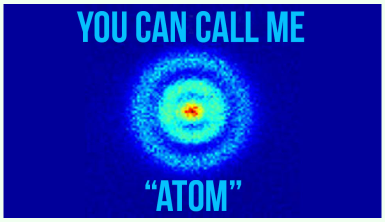
Figure 1: Don't be afraid of strong fields, but take care of pair production danger.

- Classically, by Gauss law the electron will not "feel" the Finite Size of the proton (assuming its charge distribution to be spherically symmetric). Hence, the fact that we can calculate it and

measure it is indeed an unappreciated quantum effect (of the wave function).
Is it non-local?
Can it be macroscopic? Yes, en electron around a Back Hole will know that it is a Black Hole and not a spherically symmetric mass distribution.

$$E \to E - i\frac{\Gamma}{2}$$

which means we have an unstable bound state (orbit in the macroscopic language)



- For $l = 0$, we learn that classically there is no ground state and the electron by emitting electromagnetic radiation will fall into the center. This is not true as minimum of the true potential is now the classical ground state ($\mathcal{E} \geq V = V_{eff}$). Quantum Mechanics chooses, however, another ground state.

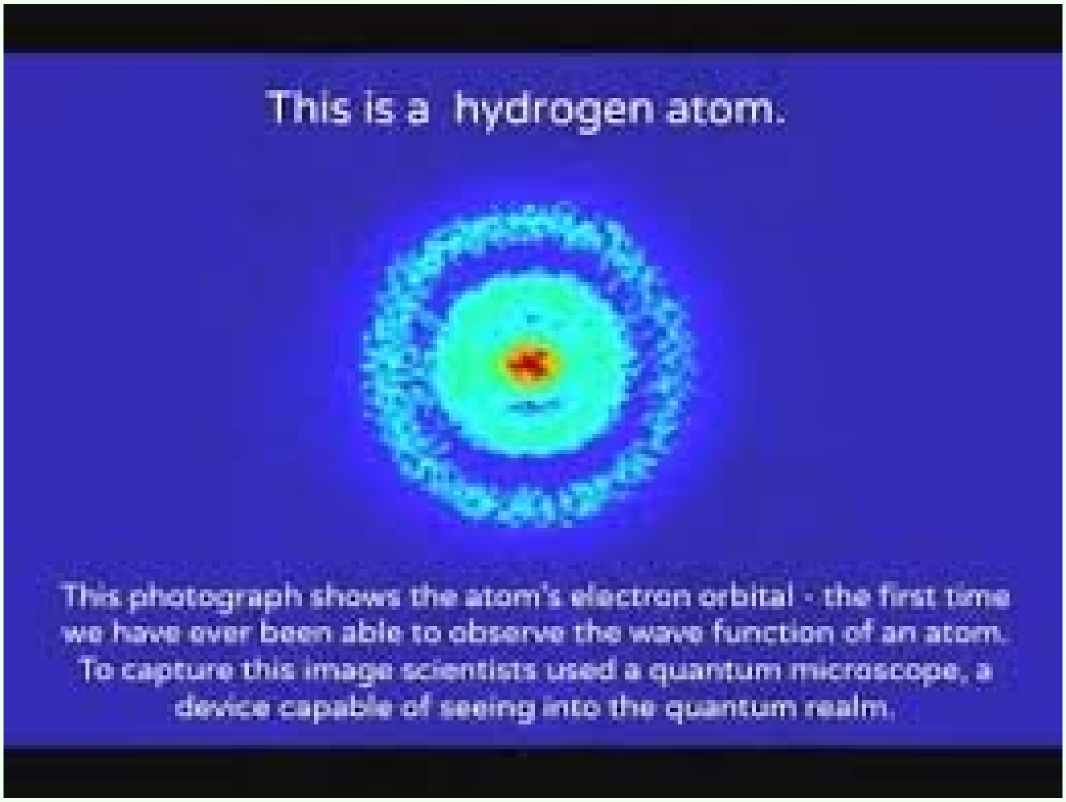


Figure 2: Smile, Hydrogen atom, you are on a quantum camera.

Selected for a Viewpoint in *Physics*
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Hydrogen Atoms under Magnification: Direct Observation of the Nodal Structure of Stark States

A. S. Stodolna,[1,*] A. Rouzée,[1,2] F. Lépine,[3] S. Cohen,[4] F. Robicheaux,[5]
A. Gijsbertsen,[1] J. H. Jungmann,[1] C. Bordas,[3] and M. J. J. Vrakking[1,2,*]
[1]FOM Institute AMOLF, Science Park 104, 1098 XG Amsterdam, Netherlands
[2]Max-Born-Institut, Max Born Straße 2A, D-12489 Berlin, Germany
[3]Institut Lumière Matière, Université Lyon 1, CNRS, UMR 5306, 10 Rue Ada Byron, 69622 Villeurbanne Cedex, France
[4]Atomic and Molecular Physics Laboratory, Physics Department, University of Ioannina, 45110 Ioannina, Greece
[5]Department of Physics, Auburn University, Auburn, Alabama 36849, USA
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To describe the microscopic properties of matter, quantum mechanics uses wave functions, whose structure and time dependence is governed by the Schrödinger equation. In atoms the charge distributions described by the wave function are rarely observed. The hydrogen atom is unique, since it only has one electron and, in a dc electric field, the Stark Hamiltonian is exactly separable in terms of parabolic coordinates (η, ξ, φ). As a result, the microscopic wave function along the ξ coordinate that exists in the vicinity of the atom, and the projection of the continuum wave function measured at a macroscopic distance, share the same nodal structure. In this Letter, we report photoionization microscopy experiments where this nodal structure is directly observed. The experiments provide a validation of theoretical predictions that have been made over the last three decades.

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The development of quantum mechanics in the early part of the last century has had a profound influence on the way that scientists understand the world. Central to quantum mechanics is the concept of a wave function that satisfies the time-dependent Schrödinger equation [1]. According to the Copenhagen interpretation, the wave function describes the probability of observing the outcome of measurements on a quantum mechanical system, such as measurements of the energy or the position or momenta of constituents [2]. The Copenhagen interpretation thus allows reconciling the occurrence of nonclassical phenomena on the nanoscale with manifestations and observations made on the macroscale, which correspond to viewing one of a number of possible realizations allowed for by the wave function.

Despite the overwhelming impact on modern electronics and photonics, understanding quantum mechanics and the many possibilities that it describes continues to be intellectually challenging, and has motivated numerous experiments that illustrate the intriguing predictions contained in the theory [3]. Using ultrafast lasers, Rydberg wave packet experiments have been performed illustrating how coherent superpositions of quantum mechanical stationary states describe electrons that move on periodic orbits around nuclei [4]. The wave function of each of these electronic stationary states is a standing wave, with a nodal pattern that reflects the quantum numbers of the state. Mapping of atomic and molecular momentum wave functions has been extensively explored by means of (e, $2e$) spectroscopy, using coincident detection of the momentum of both an ejected and a scattered electron to retrieve the momentum distribution of the former prior to ionization [5]. In the spirit of scanning tunneling methods, orbital tomography based on high harmonic generation was developed as a method allowing the determination of atomic and molecular orbitals [6,7]. In this Letter we will present experiments where the nodal structure of electronic wave functions of hydrogen atoms is measured, making use of a photoionization microscopy experiment, where photoelectrons resulting from ionization after excitation of a quasibound Stark state are measured on a two-dimensional detector.

The hydrogen is a unique atom, since it only has one electron and, in a dc electric field, the Stark Hamiltonian is exactly separable in terms of parabolic coordinates. For this reason, an experimental method was proposed about thirty years ago, when it was suggested that experiments ought to be performed projecting low-energy photoelectrons resulting from the ionization of hydrogen atoms onto a position-sensitive two-dimensional detector placed perpendicularly to the static electric field, thereby allowing the experimental measurement of interference patterns directly reflecting the nodal structure of the quasibound atomic wave function [8–10].

In a static electric field F the wave function of atomic hydrogen can be separated in terms of the parabolic coordinates η, ξ, φ ($\eta = r - z$ and $\xi = r + z$, where r is the distance of the electron from the proton, z is the displacement along the electric field axis and $\varphi = \tan^{-1}(y/x)$ is the azimuthal angle [see Fig. 1(a) and Ref. [11]]). Note that atomic units are used, unless specified otherwise. Consequently, the wave function may be written as a product of functions $\chi_1(\xi)$ and $\chi_2(\eta)$ that separately describe the dependence along ξ and η,

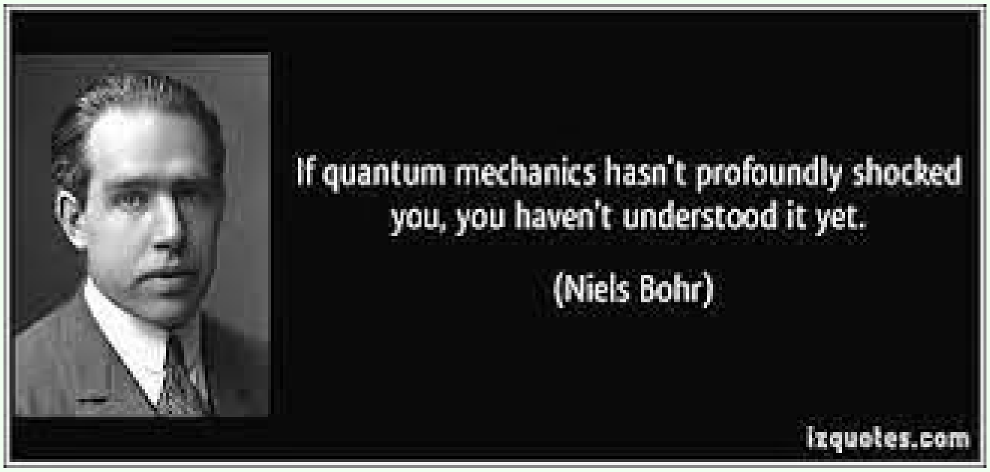


Figure 3: An electron in a hydrogen atom with a Finite Size potential and an electron around a Black Hole display a similar quantum mechanical effect.

3. The role of $\gamma\gamma$ corrections

So far we have obtained a potential by the Fourier transform of a (non-relativistic) scattering amplitude. The famous light-light "correction" follows a different logic:
Classically light does not interact with light (abelian gauge theory). Quantum Mechanics (Quantum Field Theory) introduces light-light scattering via one loop box diagram

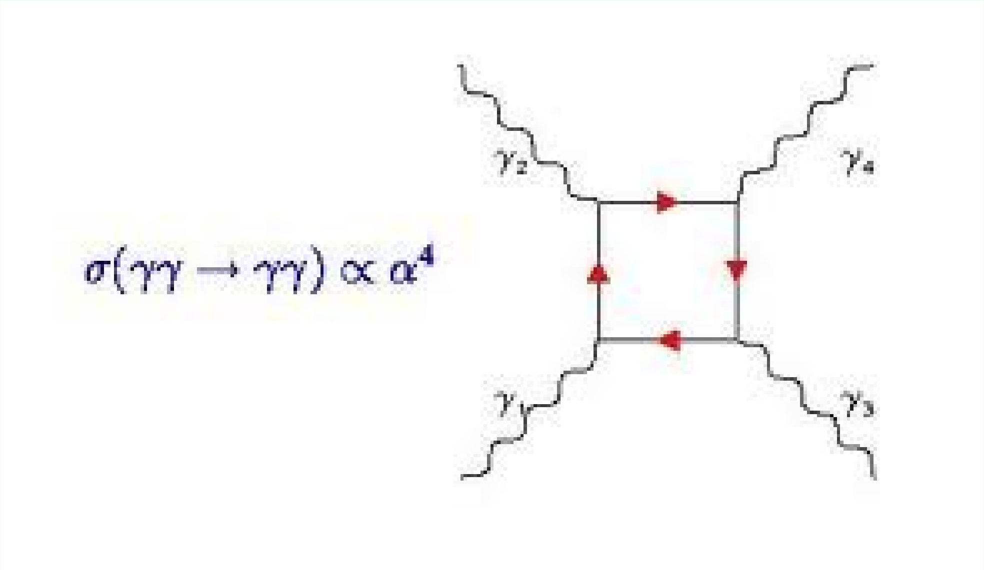


Figure 4: Light-light scattering

Effectively, this is a four-photon vertex and a new quantum effect. We can incorporate it back into the Lagrangian of Electrodynamics:

Euler-Heisenberg Theory

V. B. Berestetskii, E. M. Lifshitz and L .P. Pitaevskii, “Quantum Electrodynamics”, Landau-Lifschitz IV with contribution of Schwinger, Weisskopf and many others.

Lagrangian

The Lagrangian must be gauge invariant, hence in general a function of

$$\mathfrak{T} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} = \frac{1}{2}(\boldsymbol{E}^2 - \boldsymbol{B}^2)$$

$$\mathfrak{G} = \frac{1}{4} F_{\mu\nu} \tilde{F}^{\mu\nu} = \boldsymbol{E} \cdot \boldsymbol{B}$$

Then, we can expect that first approximation is quadratic in the invariants $\mathfrak{T}$, $\mathfrak{G}$. Indeed,

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\rm EH}$$

$$\mathcal{L}_0 = \mathfrak{T}$$

$$\mathcal{L}_{\rm EH} = \eta \left((\boldsymbol{E}^2 - \boldsymbol{B}^2)^2 + 7(\boldsymbol{E} \cdot \boldsymbol{B})^2 \right)$$

$$\propto \kappa \mathfrak{T}^2 + \lambda \mathfrak{G}^2$$

with

$$\eta = \frac{\alpha^2}{360 \pi^2 m_e^2}$$

Conditions on validity

- weak fields

$$\mathcal{L} \sim F^2(1 + \eta F^2)$$

$$F \sim E,\ B$$

$$\eta E^2,\ \eta B^2 \ll 1$$

It follows then

$$E \ll 2 \times 10^3\ \mathrm{MeV}$$

- Slow varying fields (sometimes paraphrased as constant fields)

- No pair production, .i.e.,

$$\int d^3x \boldsymbol{E}^2 \propto \mathscr{E}(\mathrm{field}) < 2m_e$$

We will come back to these conditions after solving for the electric field.

New Maxwell equations

The homogeneous Maxwell equations remain unchanged (since they define simply the electromagnetic potentials)

$$\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$$

$$\boldsymbol{\nabla} \times \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = 0$$

The inhomogeneous new Maxwell equations can be written in a form resembling the Maxwell theory in matter. Define:

$$\boldsymbol{D} \equiv \boldsymbol{E} + 4\pi \boldsymbol{P}$$

$$\boldsymbol{P} = \eta \left[4\boldsymbol{E}(\boldsymbol{E}^2 - \boldsymbol{B}^2) + 14\boldsymbol{B}(\boldsymbol{E} \cdot \boldsymbol{B}) \right]$$

$$\boldsymbol{H} \equiv \boldsymbol{B} - 4\pi \boldsymbol{M}$$

$$\boldsymbol{M} = \eta \left[-4\boldsymbol{B}(\boldsymbol{E}^2 - \boldsymbol{B}^2) + 14\boldsymbol{E}(\boldsymbol{E} \cdot \boldsymbol{B}) \right]$$

The new inhomogeneous Maxwell read now:

$$\boldsymbol{\nabla} \cdot \boldsymbol{D} = \rho$$

$$\boldsymbol{\nabla} \times \boldsymbol{H} - \frac{\partial \boldsymbol{D}}{\partial t} = \boldsymbol{j}$$

Electrostatics

Put $\boldsymbol{B} = 0$ and neglect time derivatives. Then Gauss law for $\boldsymbol{D}$ reads

$$\boldsymbol{\nabla} \cdot \boldsymbol{D} = \rho = \boldsymbol{\nabla} \cdot \boldsymbol{E}_0$$

where E_0 is the electric fields arsing in the Maxwell theory given the charge distribution (we treat the charge distribution as a given source) ρ. Hence we end up with an algebraic equations

$$\boldsymbol{E} + 4\pi \boldsymbol{P} = \boldsymbol{E} + \eta' E^3 \boldsymbol{E} = \boldsymbol{E}_0$$

where

$$\eta' = 16\pi\eta$$

For the spherical symmetric case we obtain a third order polynomial equation for the electric field $\boldsymbol{E}$ given the "standard" Maxwellian field $\boldsymbol{E}_0$

$$E + \eta' E^3 = E_0$$

The solution is $\boldsymbol{E}[\boldsymbol{E}_0]$.

Figure 5: Heisenberg, Weizsäcker and Euler

For the Coulomb field (of point-like proton), i.e., $\boldsymbol{E}_0 = e/r^2$ one can get an non-pertubative solution

$$E = \left(\frac{e}{2\eta' r^2}\right)^{1/3} \times$$

$$\left(\sqrt[3]{1+\sqrt{1+\frac{1}{27\eta'}\left(\frac{2r^2}{e}\right)^2}} + \sqrt[3]{1+\sqrt{1-\frac{1}{27\eta'}\left(\frac{2r^2}{e}\right)^2}}\right)$$

For large r one obtains the pertubative solution, linear in powers of the charge

$$E \simeq \frac{e}{r^2}\left(1 - \eta' \left(\frac{e}{r^2}\right)^2\right)$$

For small r the behaviour is softer than $1/r$ i.e.

$$E \simeq \left(\frac{e}{\eta' r}\right)^{2/3}$$

This approximation is equivalent to neglect the linear terms in the cubic equations for the field (strong fields).

Extended charge distribution

Taking now $\boldsymbol{E}_0 = \boldsymbol{E}_p$ where $\boldsymbol{E}_p$ is the proton electric field including the form-factor effects, we arrive at

$$E = \left(\frac{E_p}{2\eta'}\right)^{1/3} \times$$

$$\left(\sqrt[3]{1+\sqrt{1+\frac{4}{27\eta' E_p^2}}}+\sqrt[3]{1+\sqrt{1-\frac{1}{27\eta' E_p^2}}}\right)$$

Again for strong fields (small distances) one would expect that $E \propto (E_p)^{2/3}$, i.e., the field becomes weaker.

Effects of Higher loops

Before presenting the results it is instructive to look at the effect of higher loops: two loops in
B. Körs and M. G. Schmidt, Eur. Phys. J. **C6** (1999) 175
The polynomial equation for E is now a quintic

$$E + \eta_1 E^3 + \eta_2 E^5 = E_0$$

where $\eta_1 \simeq \eta'$.

Effects of $\gamma\gamma$ corrections

The energy content of the electric field:

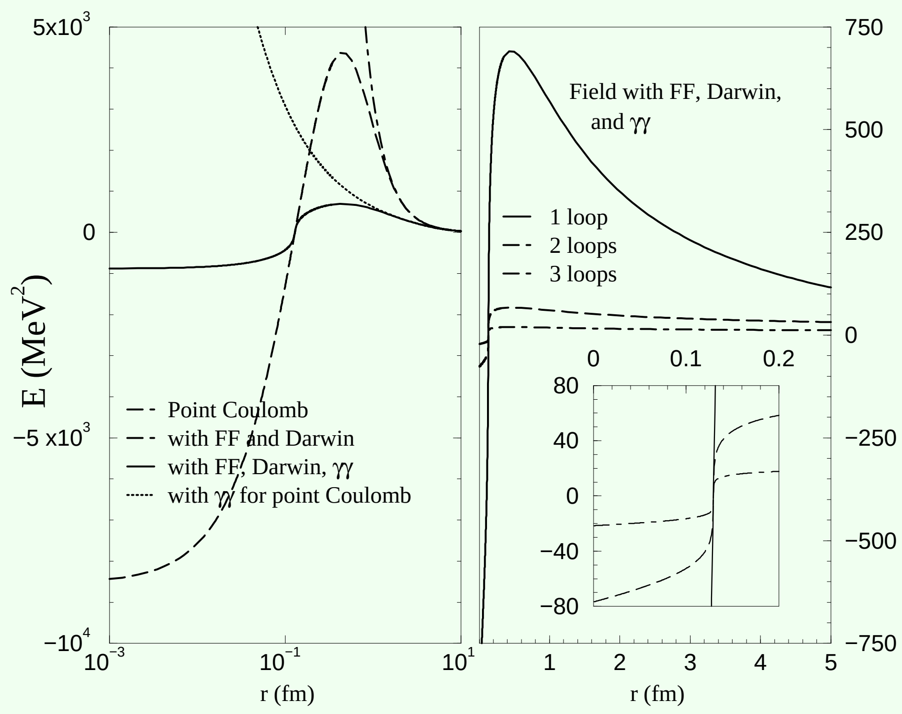
$$\mathscr{E}[E_p] \simeq 1\ MeV$$

$$\mathscr{E}[E_{\gamma\gamma,1loop}] \simeq 0.26\ MeV$$

$$\mathscr{E}[E_{\gamma\gamma,2loop}] \simeq 0.076\ MeV$$

where $E_{\gamma\gamma} = E[E_p]$.One can see that the loop results are well below the pair production threshold.

Field strength



For small distances the light-light contribution reduces the field strength considerably. The "3-loop" result is an educated guess. i.e. by dimensional analysis (there is only one scale, the electron mass) and by properly introducing the powers of α and by guessing the rest of the numerical factors we wrote a polynomial equation of seventh order for E if the effect saturates.

3. Consequences for the energy levels

Recall the formula of the Finite Size correction to the energy levels within the framework of the Maxwell theory

$$\Delta\mathcal{E} = \frac{e}{6}|\Psi(0)|^2 \int d^3x r^2 \boldsymbol{\nabla} \cdot \boldsymbol{E}_p$$

with $\boldsymbol{\nabla} \cdot \boldsymbol{E}_p = \rho$. In the Euler-Heisenberg theory $\boldsymbol{\nabla} \cdot \boldsymbol{E}_{\gamma\gamma} \neq \rho$ and one gets with $E_{\gamma\gamma} = E[E_p]$

$$\Delta\mathcal{E} = \frac{e}{6}|\Psi(0)|^2 \int d^3x r^2 \boldsymbol{\nabla} \cdot \boldsymbol{E}_{\gamma\gamma}$$

Now from our polynomial equation for the electric field

$$\boldsymbol{E} + \eta_1 \boldsymbol{E} E^2 + \eta_2 \boldsymbol{E} E^4 = \boldsymbol{E}_p$$

we can get $\boldsymbol{\nabla} \cdot \boldsymbol{E}$ ($\boldsymbol{E} = \boldsymbol{E}_{\gamma\gamma}$) as

$$\boldsymbol{\nabla} \cdot \boldsymbol{E} = \frac{\rho + 4\eta_2 \boldsymbol{E} \cdot \boldsymbol{\nabla} E + 2\eta_1 \boldsymbol{E} \cdot \boldsymbol{\nabla} E}{\eta_1 E^2 + \eta_1 E^4 + 1}$$

using the fact $\boldsymbol{\nabla} \cdot \boldsymbol{E}_p = \rho$ One would be tempted to assume

$$\eta_2 E^4 + \eta_1 E^2 \ll 1$$

In such a case the first term of the divergence would be the the charge distribution and

$$\Delta \mathcal{E} = \frac{e}{6} |\Psi(0)|^2 < r^2 > + ...$$

One could handle theoretically the other contributions and the charged proton radius would be, in principle, “measurable” from spectroscopy. However, the requirement of the denominator of the divergence being small imposes

$$E \ll 300 \ \ MeV^2$$

in one loop and

$$E \ll 23 \ MeV^2$$

in two loop approximation. Both these inequalities are not satisfied and therefore it seems that we cannot disentangle the Finite Size Correction (FSC) from the $\gamma\gamma$ correction.

$$\Delta\mathcal{E}(FSC) \simeq 4.1 \times 10^{-9}\ eV$$

$$\Delta\mathcal{E}(FSC + \gamma\gamma) \simeq 8.54 \times 10^{-8}\ eV$$

$$\Delta\mathcal{E}(point - like\ \gamma\gamma) \simeq 8.50 \times 10^{-8}\ eV$$

If we take the difference of the last two equations as a rough measure of the FSC in the Euler-Heisenberg theory then its importance is one order of magnitude less than in the Maxwell theory.

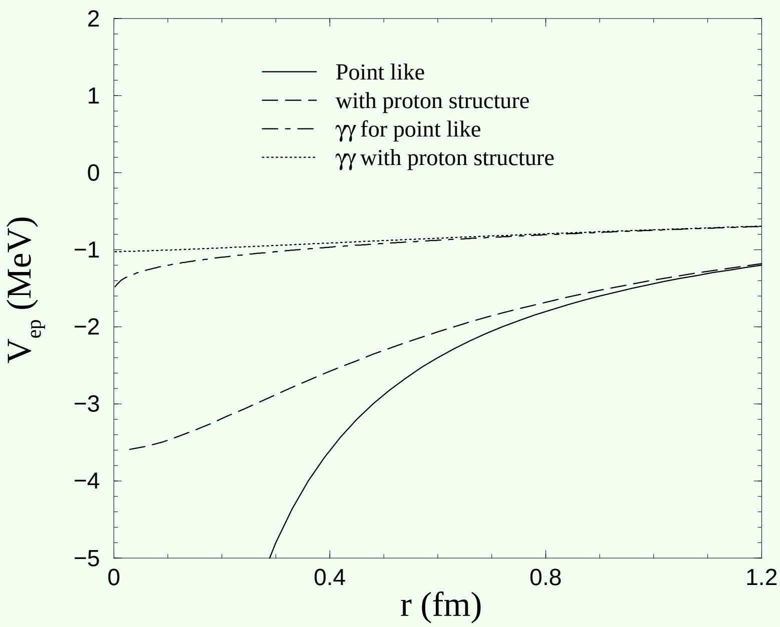
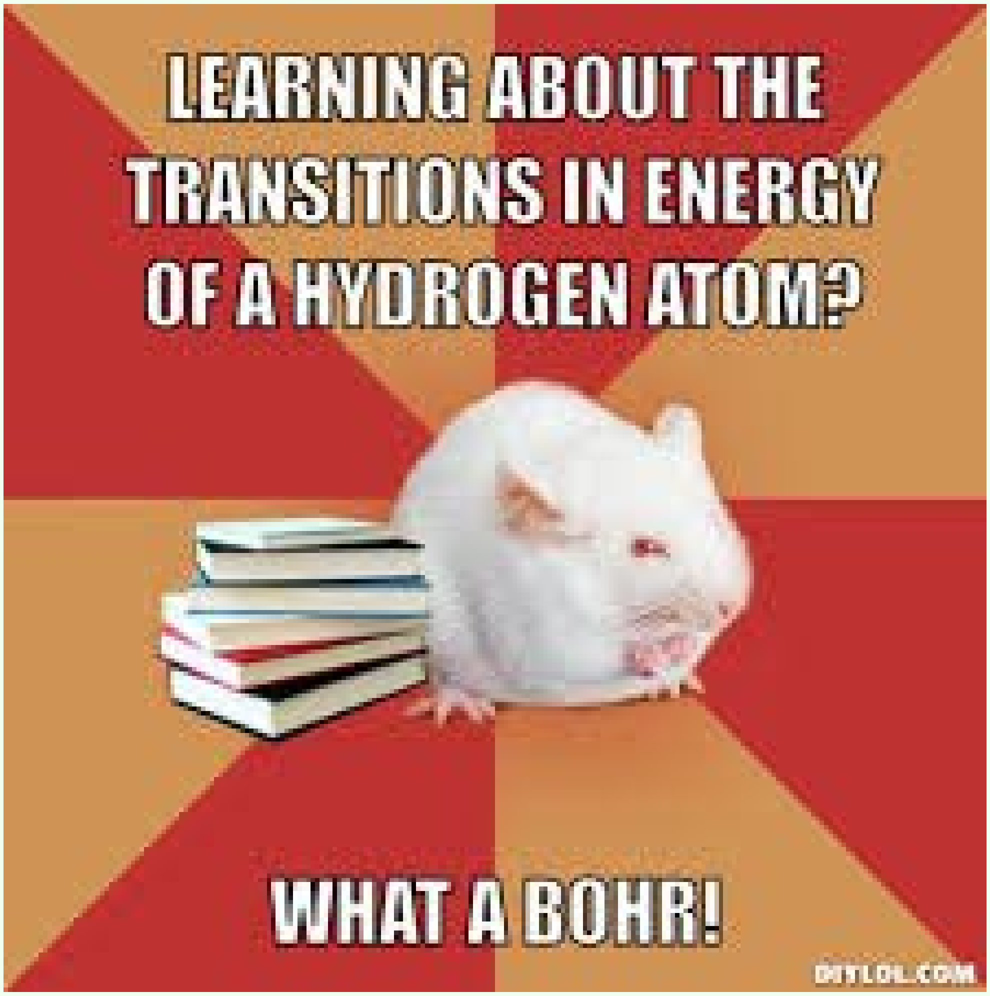


Figure 6: $\Delta\mathcal{E} \propto \int d^3x|\Psi(x)|^2(V + e/r)$. **The effect is: the smaller** $|V|$ **the bigger the correction.**



Where could this be relevant?

$\Delta\mathcal{E}$ with Finite Size Corrections (FSC) is the simplest expression with FSC in the hydrogen atom. Already here the FSC could not be disentangled from the light-light contribution. There are FSC's also for other levels and transitions like, e.g., hyperfine interaction (spin-spin) with claims of unprecedented precision.

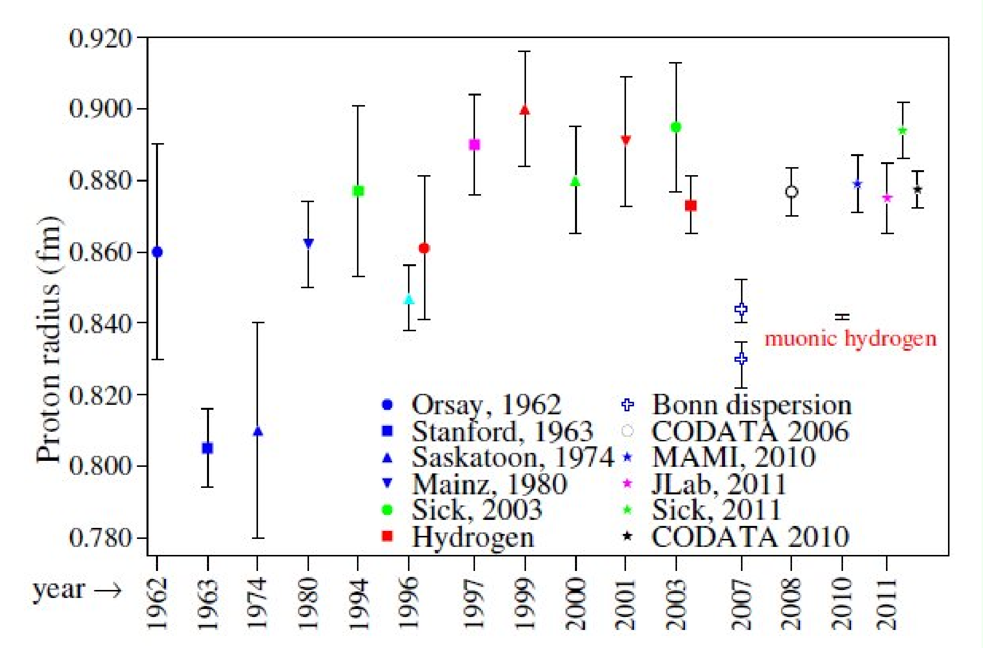


Figure 1: Proton radius determinations over time. Electronic measurements seem to settle around r_p=0.88 fm, whereas the muonic hydrogen value [1] is at 0.84 fm.

Figure 7: New York Times, Spiegel etc reported on “Honey, I shrank the proton”

Figure 8: To extract static properties of the proton from spectroscopy is an especially "theory dependent measurement".

4. Outlook

- Beyond the electric potential of the proton: e.g. The electron Darwin term

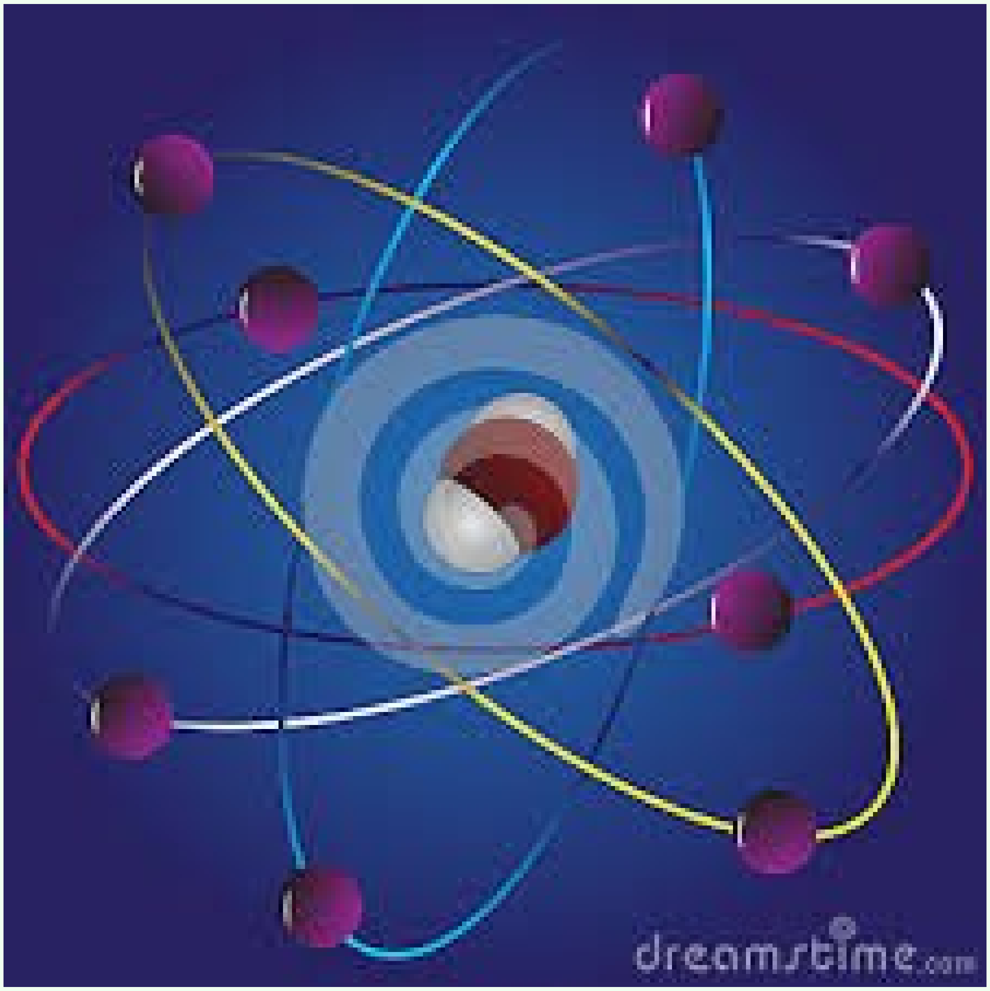
$$V_{ep}^{\gamma\gamma} = eV_{p}^{\gamma\gamma} + \frac{e}{8m_e^2}\boldsymbol{\nabla} \cdot \boldsymbol{E}_{\gamma\gamma}$$

This would be supported by the Dirac equation where the potential is given from "outside".

$$V_{ep}^{\gamma\gamma} = eV_{p}^{\gamma\gamma} + \frac{e}{8m_e^2}\rho$$

This would be supported by the Breit equation.

- More complicated transitions

- 

Other nuclei

$$^{Z}_{A}\rho \rightarrow ^{Z}_{A} E \equiv E_0 \rightarrow ^{Z}_{A} E_{\gamma\gamma} = E[E_0]$$

Figure 9: UNESCO has declared 2015 as the Year of Light.

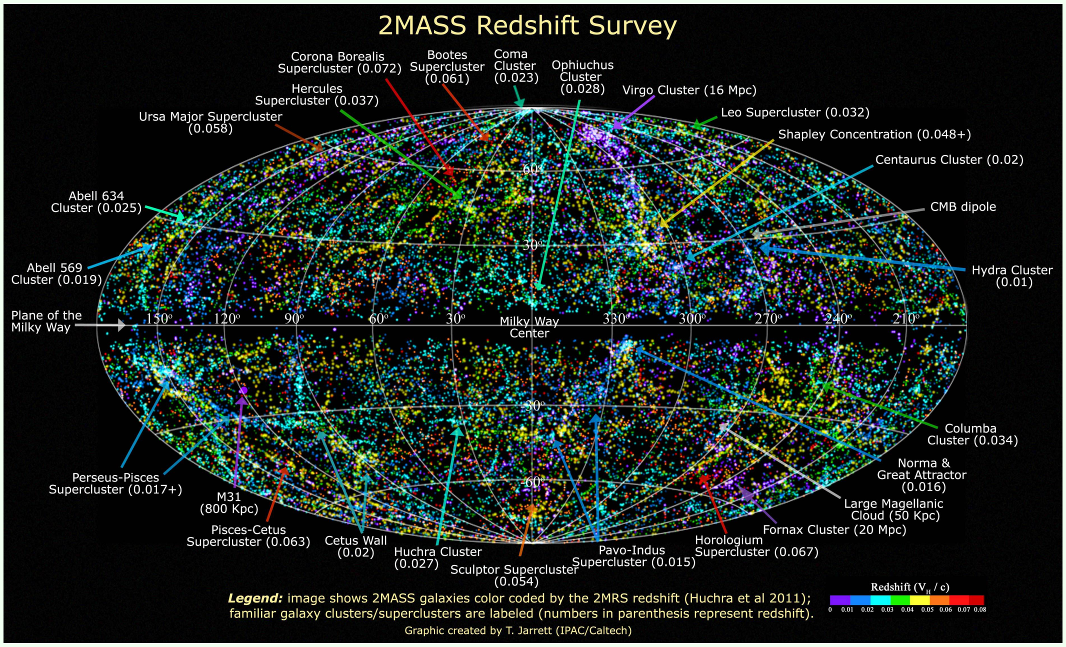


Figure 10: Light from Mega parsecs

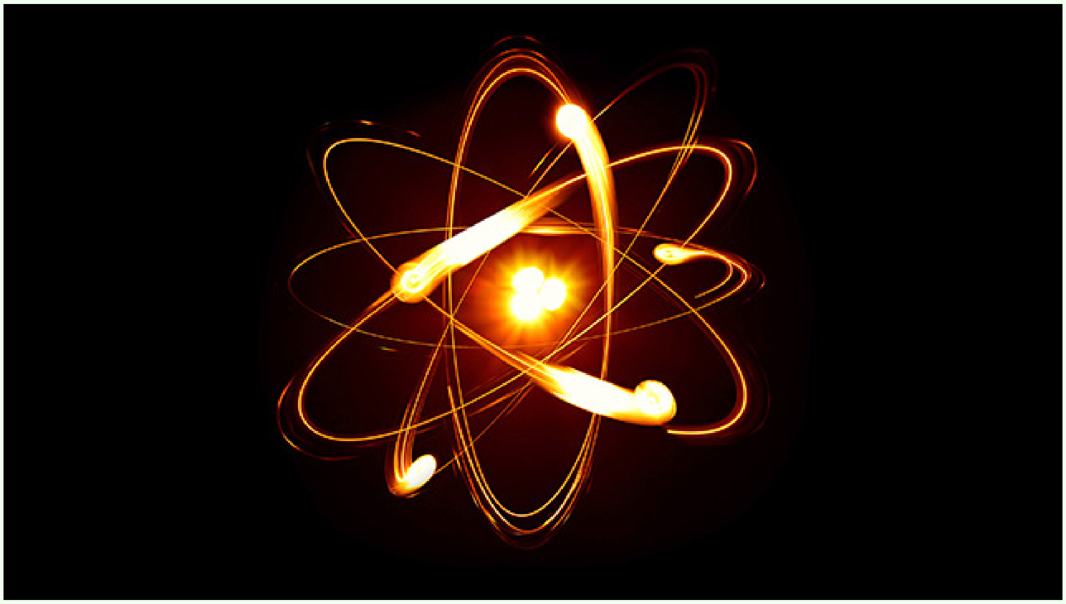


Figure 11: and light from the atoms are, of course, connected. We argued that the quantum mechanical correction leading to light-light interaction might change our picture of the atoms at very small distances. This might also change the way how we handle the correction to the energy levels in the hydrogen atom.

T. H. Huxley: "The great tragedy of science - the slaying of a beautiful hypothesis by an ugly fact."

THANK YOU!