Lamb Shift and Sub-Compton Electron Dynamics: Dirac Hydrogen Wavefunctions without Singularities

Lloyd Watts

October 16, 2015

Introduction

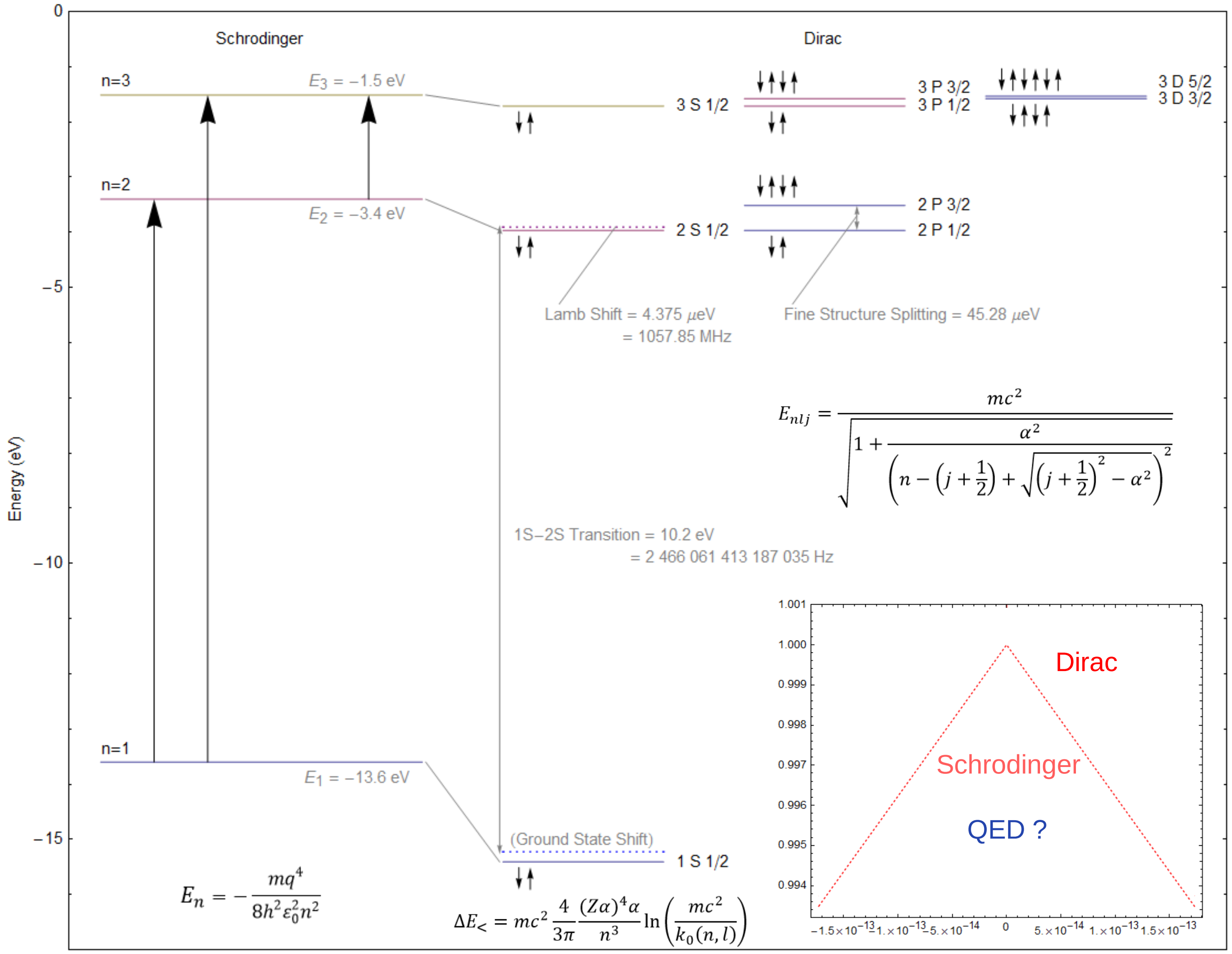
Schrodinger Hydrogen Atom explains basic energy levels, but does not explain spin or fine structure, and has wavefunctions with cusps at origin.

Dirac Hydrogen Atom explains spin and fine structure and anti-matter, but does not explain Lamb Shift, and has wavefunctions with singularities at origin.

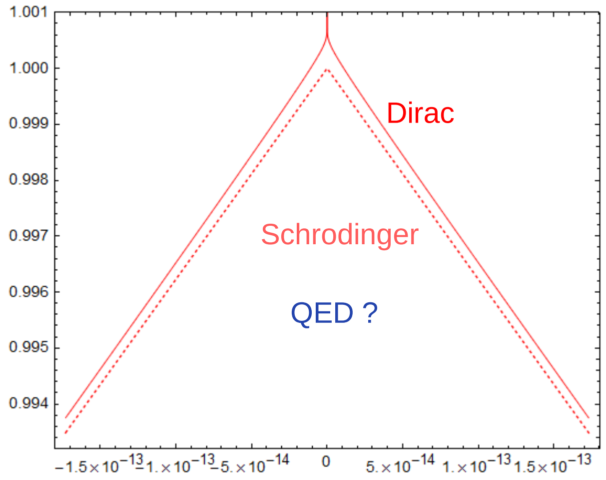
QED explains Lamb Shift, but is silent about wavefunctions.

Can we find the QED-compatible wavefunction?

Energy Levels for Atomic Hydrogen



Why seek the QED-compatible wavefunction?



Pedagogical: The Hydrogen Atom story is not complete without it. Currently we have the Dirac wavefunction with singularity (Darwin, 1928), and even though QED gets Lamb Shift (1948), the literature has never gone back to correct the singular Dirac wavefunction problem.

Revealing of Electron Dynamics: A QED-compatible Dirac wavefunction may reveal something about bound and free electron dynamics that is not yet understood, since the focus has been on accuracy of spectral energy and not spatial dynamics.

Revealing of Quantum Transition Dynamics: A QED-compatible Dirac wavefunction may be necessary to understand the dynamics of a quantum transition, where a breakdown of prevailing assumptions and deeper physics could be seen in non-observable regions (c.f. Watts, 2000 JASA, Mode-Coupling Liouville-Green Solution for Cochlear Mechanics).

Schrodinger Hydrogen Atom

$$\frac{\hbar^2}{2m}\nabla^2\psi(r,\theta,\phi) + \big(E - V(r)\big)\psi(r,\theta,\phi) = 0$$

$$V(r) = -\frac{q^2}{4\pi\varepsilon_0 r} = -\frac{\hbar^2}{m a_0 r}$$

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi),$$

$$R''(r) + \frac{2}{r}R'(r) + \left(\frac{2m}{\hbar^2}\big(E - V(r)\big) - l(l+1)\right)R(r) = 0$$

Point Charge Assumption
Singular Coulomb Potential
Leads to cusp in solution

$$E_n = -\frac{mq^4}{8h^2\varepsilon_0^2 n^2} = -\frac{\hbar^2}{2ma_0^2 n^2}$$

State	Normalized Radial Solution	Normalized Wavefunction Solution
1S	$R_{1S}(r) = \frac{2}{{a_0}^{3/2}} e^{-\frac{r}{a_0}}$	$\psi_{1S}(r) = \frac{1}{\sqrt{\pi}{a_0}^{3/2}} e^{-\frac{r}{a_0}}$
2S	$R_{2S}(r) = \frac{1}{2\sqrt{2}{a_0}^{3/2}}\left(2 - \frac{r}{a_0}\right) e^{-\frac{r}{2a_0}}$	$\psi_{2S}(r) = \frac{1}{4\sqrt{2\pi}{a_0}^{3/2}}\left(2 - \frac{r}{a_0}\right) e^{-\frac{r}{2a_0}}$
2P	$R_{2P}(r) = \frac{1}{2\sqrt{6}{a_0}^{3/2}} \frac{r}{a_0} e^{-\frac{r}{2a_0}}$	$\psi_{2P}(r) = \frac{1}{4\sqrt{2\pi}{a_0}^{3/2}} \frac{r\cos\theta}{a_0} e^{-\frac{r}{2a_0}}$

Dirac Hydrogen Atom

$$\left(-c\left(\alpha_x p_x + \alpha_y p_y + \alpha_z p_x\right) - \beta mc^2\right)\Psi + \left(E - V(r)\right)\Psi = 0$$

$$V(r) = -\frac{q^2}{4\pi\varepsilon_0 r} = -\frac{\hbar^2}{ma_0 r}$$

$$\alpha_x = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \quad \alpha_y = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}, \quad \alpha_z = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}, \quad \beta = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix},$$

$$\Psi(r,\theta,\phi) = \begin{pmatrix} \phi(r,\theta,\phi) \\ \chi(r,\theta,\phi) \end{pmatrix} = \begin{pmatrix} f(r)\Omega_{jlm}(\theta,\phi) \\ (-1)^{\frac{1}{2}(1+l-l')}\, g(r)\Omega_{jl'm}(\theta,\phi) \end{pmatrix},$$

Point Charge Assumption
Singular Coulomb Potential
Leads to Singularity in solution

$$E_{nlj} = \frac{mc^2}{\sqrt{1 + \frac{\alpha^2}{\left(n - \left(j + \frac{1}{2}\right) + \sqrt{\left(j + \frac{1}{2}\right)^2 - \alpha^2}\right)^2}}}$$

$$f'(r) + \frac{1+\kappa}{r} f(r) - \frac{1}{\hbar c}\left(E + mc^2 - V(r)\right)g(r) = 0$$

$$g'(r) + \frac{1-\kappa}{r} g(r) + \frac{1}{\hbar c}\left(E - mc^2 - V(r)\right)f(r) = 0$$

$$E_{1S½} = mc^2\sqrt{1 - \alpha^2}$$

$$f_{1S½}'(r) - \left(\frac{1 + \sqrt{1-\alpha^2}}{\alpha a_0} + \frac{\alpha}{r}\right) g_{1S½}(r) = 0$$

$$g_{1S½}'(r) + \frac{2}{r}\, g_{1S½}(r) + \left(\frac{-1 + \sqrt{1-\alpha^2}}{\alpha a_0} + \frac{\alpha}{r}\right) f_{1S½}(r) = 0$$

$$f_{1S½}(\infty) = 0$$

$$g_{1S½}(\infty) = 0$$

$$\int_0^\infty \left(f_{1S½}(r)^2 + g_{1S½}(r)^2\right) r^2\, dr = 1$$

$$\Psi_{1S½down} = \frac{1}{\sqrt{\pi}{a_0}^{3/2}} e^{-\frac{r}{a_0}} \left(\frac{2r}{a_0}\right)^{-1+\sqrt{1-\alpha^2}} \sqrt{\frac{1+\sqrt{1-\alpha^2}}{\Gamma\left(1+2\sqrt{1-\alpha^2}\right)}} \begin{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ \frac{\alpha}{1+\sqrt{1-\alpha^2}} \begin{pmatrix} i\, e^{-i\phi} \sin\theta \\ -i\cos\theta \end{pmatrix} \end{pmatrix}$$

$$\Psi_{1S½up} = \frac{1}{\sqrt{\pi}{a_0}^{3/2}} e^{-\frac{r}{a_0}} \left(\frac{2r}{a_0}\right)^{-1+\sqrt{1-\alpha^2}} \sqrt{\frac{1+\sqrt{1-\alpha^2}}{\Gamma\left(1+2\sqrt{1-\alpha^2}\right)}} \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \frac{\alpha}{1+\sqrt{1-\alpha^2}} \begin{pmatrix} i\cos\theta \\ i\, e^{i\phi} \sin\theta \end{pmatrix} \end{pmatrix}$$

Quantum Electrodynamics (QED)

From Eides, Grotch, and Shelyuto (2007):

According to QED an electron continuously emits and absorbs virtual photons and as a result its electric charge is spread over a finite volume instead of being pointlike:

$$\langle r^2 \rangle = -6 \frac{dF_1(-\boldsymbol{k}^2)}{d\boldsymbol{k}^2}_{|\boldsymbol{k}^2=0} \approx \frac{2\alpha}{\pi m^2} \ln \frac{m}{\rho} \approx \frac{2\alpha}{\pi m^2} \ln(Z\alpha)^{-2}$$

The finite radius of the electron generates a correction to the Coulomb potential:

$$\delta V = \frac{1}{6}\langle r^2 \rangle \Delta V = \frac{2\pi}{3} Z\alpha \langle r^2 \rangle \delta(\boldsymbol{r})$$

The respective correction to the energy levels is simply given by the matrix element of this perturbation. The finite size of the electron leads to a shift of the hydrogen energy levels.

But notice, this informal description only gives the mean-squared radius of the electric charge spread, not the detailed charge distribution.

What is the charge distribution of the electron, consistent with Lamb Shift?

Charge Distribution → Modified Coulomb Potential → Modified Wavefunction

Charge Distribution of the Electron Candidate #1: Charged Shell

From Hestenes (2010):

- Use Space-Time Algebra to reformulate Dirac Solution in canonical form:

$$\psi = \left(\rho e^{i\beta}\right)^{\frac{1}{2}} R$$

- Electron moves on a helical path with radius $r_z = \frac{\lambda\!\!\!^{-}_c}{2}$, where $\lambda\!\!\!^{-}_C = \frac{\hbar}{mc}$ is the Reduced Compton Wavelength of the electron.

We further explore this idea:

- As electron moves around Hydrogen nucleus in spin-1/2 precessing motion, it appears as a charged shell of radius r_z .
- This leads to a Charge Distribution of

$$\rho(r) = \frac{q}{4\pi r_Z^2}\delta(r - r_Z).$$

- and a Modified Coulomb Potential (Cutoff Coulomb, Wannier 1943) of

$$V_{mod}(r) = -\frac{q^2}{4\pi\varepsilon_0 \, \mathrm{Max}(r, r_Z)}$$

- which agrees with Lamb Shift when

$$r_Z \approx \frac{\lambda\!\!\!^{-}_C}{2}(0.38126)$$

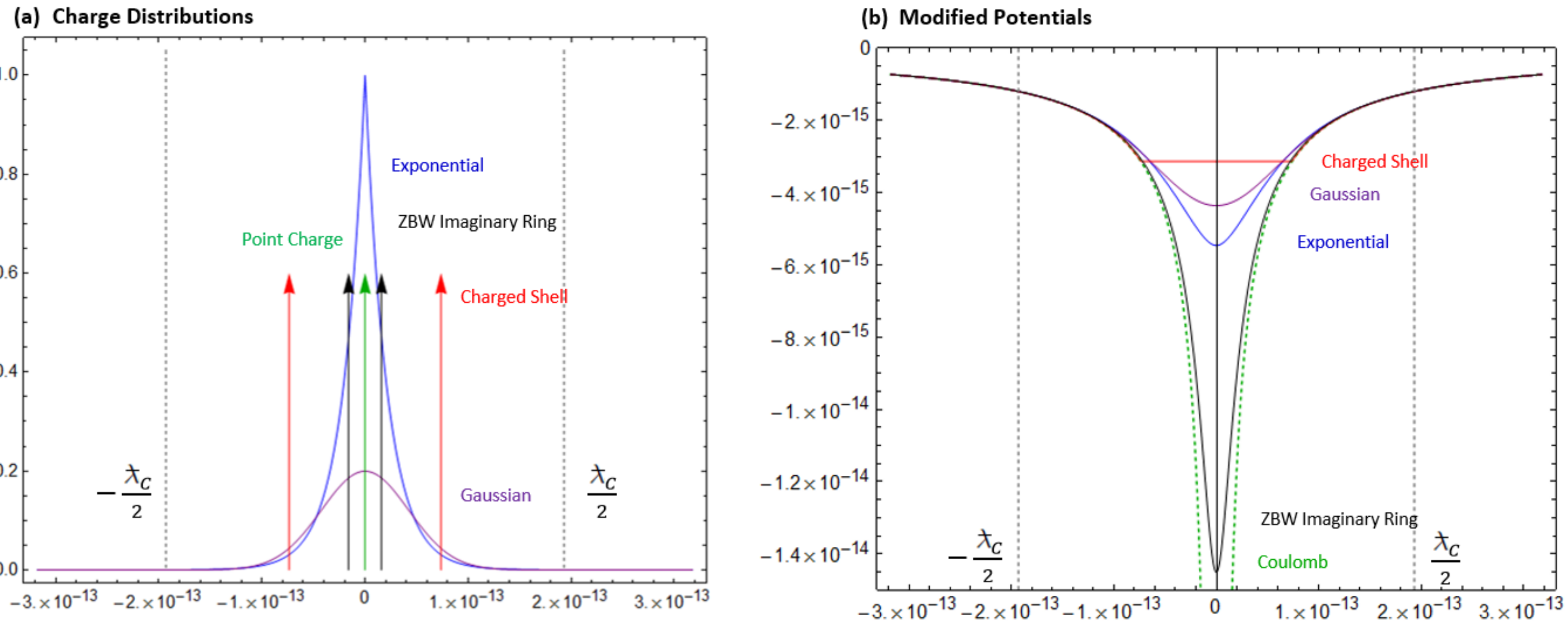
Smaller than Hestenes expected (?) by a factor of 2.62

Hestenes did not discuss Lamb Shift compatibility

Charge Distribution of the Electron: Candidates

Charge Distribution Type	Charge Distribution and Modified Coulomb Potential	Characteristic Radius to match Lamb Shift
Point Charge	$\rho(r) = q\delta(r)$ $V(r) = -\frac{q^2}{4\pi\varepsilon_0 \mathrm{r}}$	n/a
Charged Shell	$\rho(r) = \frac{q}{4\pi r_Z^2}\delta(r - r_Z)$ $V_{mod}(r) = -\frac{q^2}{4\pi\varepsilon_0 \,\mathrm{Max}(r, r_Z)}$	$r_Z \approx \frac{\lambda_C}{2}(0.38126)$
Zitterbewegung Imaginary Ring	$\rho(r) = \frac{q}{4\pi r_Z^2}\delta(r - ir_Z)$ $V_{mod}(r) = -\frac{q^2}{4\pi\varepsilon_0\sqrt{r^2 + r_Z{}^2}}$	$r_Z \approx \frac{\lambda_C}{2}(0.082364)$
Gaussian Charge Density	$\rho(r) = \frac{q}{2\sqrt{2}\pi^{3/2} r_Z^3}\, e^{-\frac{r^2}{2r_Z^2}}$ $V_{mod}(r) = -\frac{q^2}{4\pi\varepsilon_0 r}\mathrm{Erf}\left(\frac{r}{\sqrt{2}\, r_Z}\right)$	$r_Z \approx \frac{\lambda_C}{2}(0.21885)$
Exponential Charge Density	$\rho(r) = \frac{q}{\pi r_Z^3} e^{-\frac{2r}{r_Z}}$ $V_{mod}(r) = -\frac{q^2}{4\pi\varepsilon_0 r}\left(1 - e^{-\frac{2r}{r_Z}}\left(1 + \frac{r}{r_Z}\right)\right)$	$r_Z \approx \frac{\lambda_C}{2}(0.21885)$

Charge Distribution of the Electron: Candidates



ALL charge distribution candidates must fit inside the Half-Reduced Compton Radius to match Lamb Shift.

ALL charge distribution candidates tame the singularity of the Coulomb potential.

Lamb Shift is the result of Sub-Compton Electron Dynamics.

Numerical Solution for Modified Wavefunction

Given a Charge Distribution (i.e., Gaussian) and its Modified Coulomb Potential, can we find the Modified Dirac Hydrogen Wavefunction?

Hammerling (2010) developed Two-Sided Shooting Method to solve Sturm-Liouville problems on semi-infinite domains, and the Schrodinger Hydrogen problem in particular.

We extended that approach to solve the Dirac Hydrogen problem with Modified Coulomb Potential.

Original Problem

$$E_{1S\frac{1}{2}} = mc^2\sqrt{1-\alpha^2}$$

$$f_{1S\frac{1}{2}}{}'(r) - \left(\frac{1+\sqrt{1-\alpha^2}}{\alpha a_0} + \frac{\alpha}{r}\right) g_{1S\frac{1}{2}}(r) = 0$$

$$g_{1S\frac{1}{2}}{}'(r) + \frac{2}{r}\, g_{1S\frac{1}{2}}(r) + \left(\frac{-1+\sqrt{1-\alpha^2}}{\alpha a_0} + \frac{\alpha}{r}\right) f_{1S\frac{1}{2}}(r) = 0$$

$$f_{1S\frac{1}{2}}(\infty) = 0$$

$$g_{1S\frac{1}{2}}(\infty) = 0$$

$$\int_0^\infty \left(f_{1S\frac{1}{2}}(r)^2 + g_{1S\frac{1}{2}}(r)^2\right) r^2\, dr = 1$$

Modified Problem

$$\begin{aligned} E_{1S\frac{1}{2}m} &= \left(E_{1S\frac{1}{2}} - mc^2\right)\left(1+\varepsilon_{1S\frac{1}{2}}\right) + mc^2 \\ &= mc^2\left(1 + \left(-1+\sqrt{1-\alpha^2}\right)\left(1+\varepsilon_{1S\frac{1}{2}}\right)\right) \\ &= mc^2\left(\sqrt{1-\alpha^2} + \varepsilon_{1S\frac{1}{2}}\left(-1+\sqrt{1-\alpha^2}\right)\right) \end{aligned}$$

$$f_{1S\frac{1}{2}m}'(r) - \left(\frac{1+\sqrt{1-\alpha^2}+\varepsilon_{1S\frac{1}{2}}\left(-1+\sqrt{1-\alpha^2}\right)}{\alpha a_0} + \frac{\alpha}{r} A_{1S\frac{1}{2}}(r)\right) g_{1S\frac{1}{2}m}(r) = 0$$

$$g_{1S\frac{1}{2}m}'(r) + \frac{2}{r}\, g_{1S\frac{1}{2}m}(r) + \left(\frac{-1+\sqrt{1-\alpha^2}+\varepsilon_{1S\frac{1}{2}}\left(-1+\sqrt{1-\alpha^2}\right)}{\alpha a_0} + \frac{\alpha}{r} A_{1S\frac{1}{2}}(r)\right) f_{1S\frac{1}{2}m}(r) = 0$$

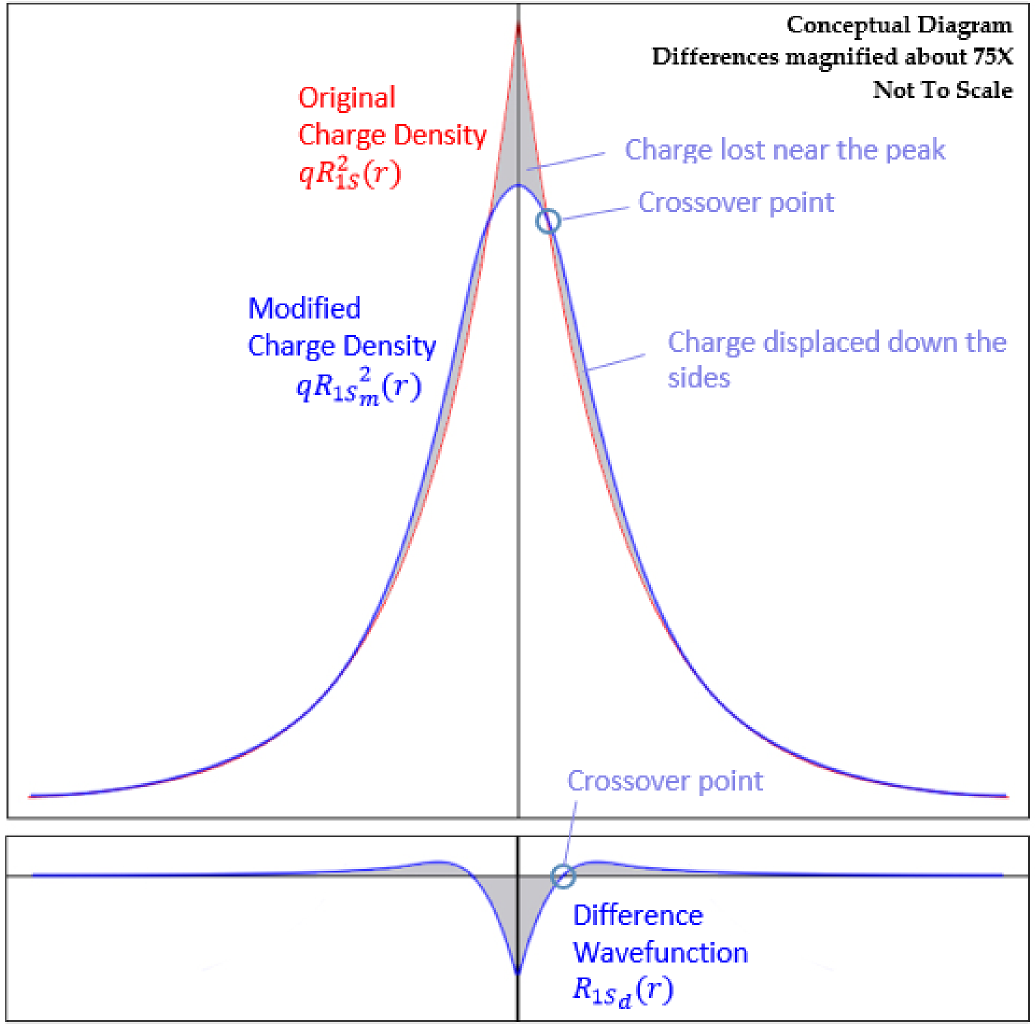
$$A_{1S\frac{1}{2}}(r) = \frac{V_{1S\frac{1}{2}}(r)}{V(r)} = \mathrm{Erf}\left(\frac{r}{\sqrt{2}\, r_Z}\right)$$

$$f_{1S\frac{1}{2}m}(\infty) = 0$$

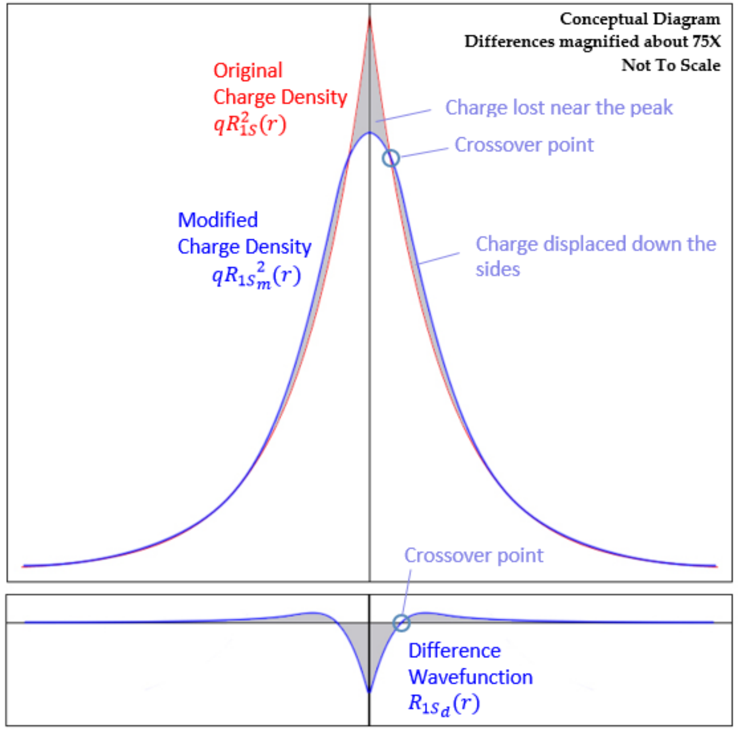
$$g_{1S\frac{1}{2}m}(\infty) = 0$$

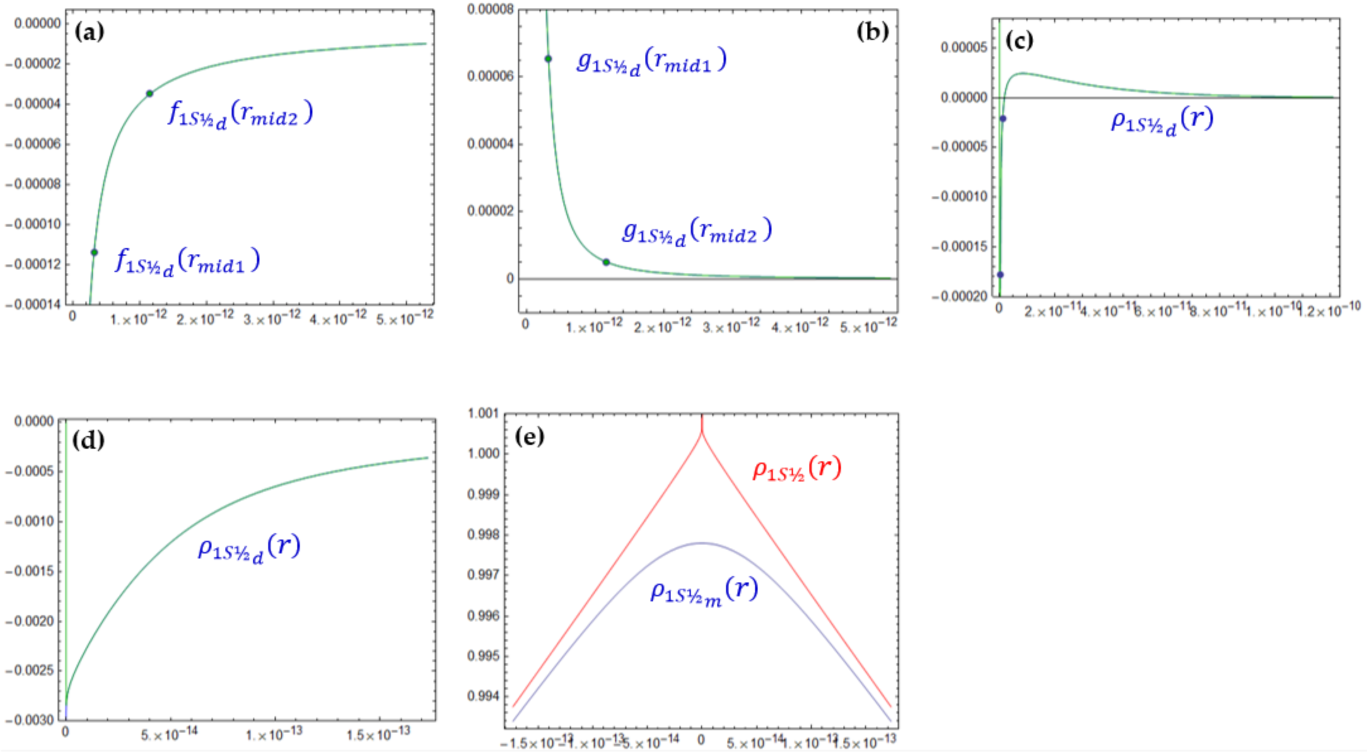
$$\int_0^\infty \left(f_{1S\frac{1}{2}m}(r)^2 + g_{1S\frac{1}{2}m}(r)^2\right) r^2\, dr = 1$$

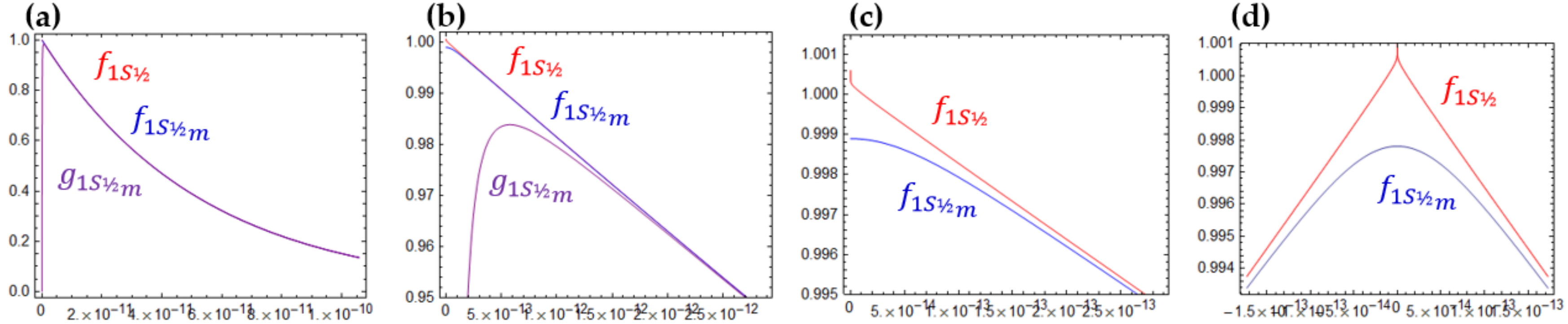
Numerical Solution for Modified Wavefunction



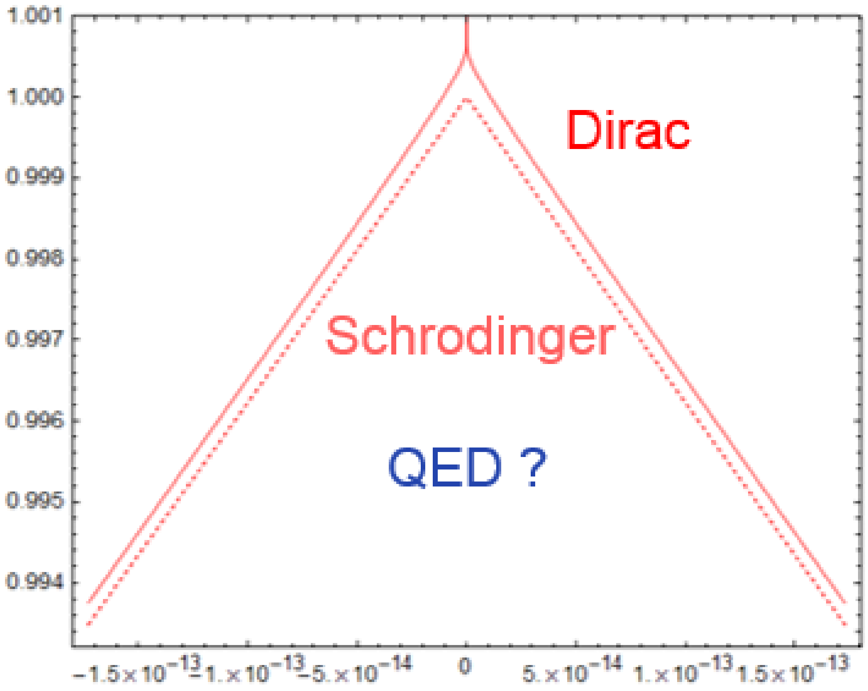
Numerical Solution for Modified Wavefunction





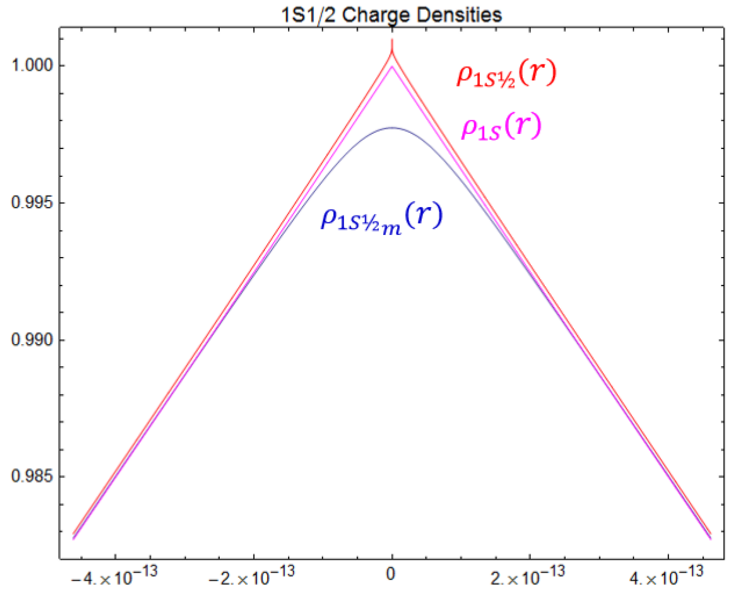


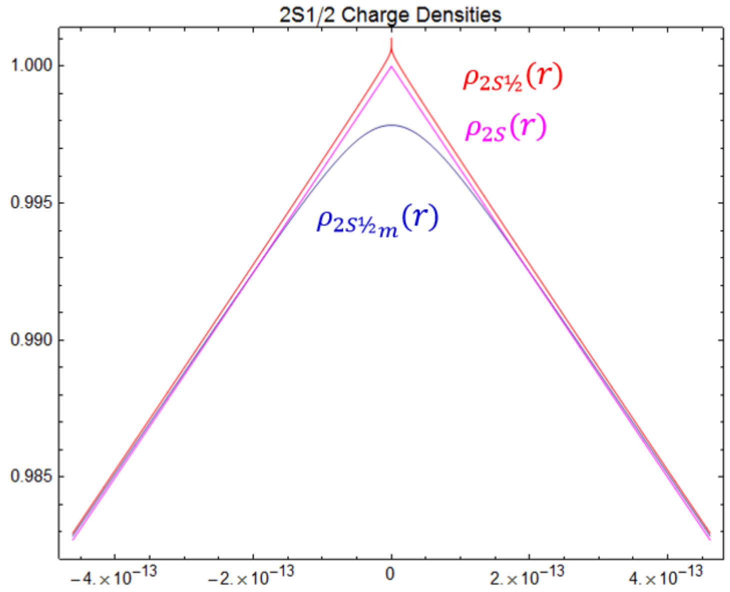
Numerical Solution for Modified Wavefunction



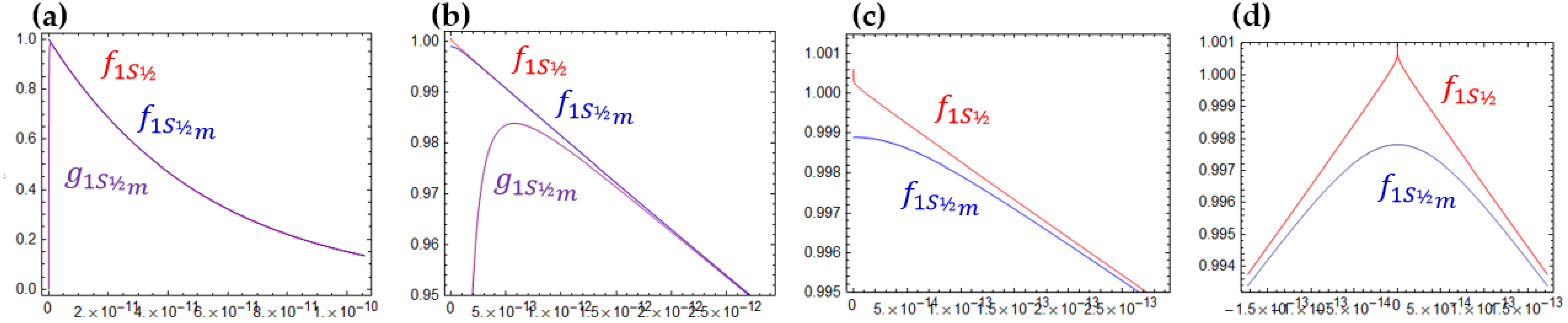
Numerical Solution for Modified Wavefunction

Charge Density has “rounded top” at origin – no cusp, no singularity.





Large Component has “rounded top” at origin, Small Component driven to zero at origin.



Discussion

Exponential Charge Distribution leads to same behavior as Gaussian:
rounded top, small component driven to zero at origin.

Same behavior expected for other distributions (Charged Shell, Imaginary Ring).

I believe this is a general result that will hold, regardless of particular charge distribution shape.

Good analytic approximations found using Confluent Hypergeometric Functions.

Implications for a Free Electron

Existing QED theory for the leading (non-relativistic) term of the Lamb Shift is

$$\Delta E_{<} = mc^2 \frac{4}{3\pi} \frac{(Z\alpha)^4 \alpha}{n^3} \ln\left(\frac{mc^2}{k_0(n,l)}\right)$$

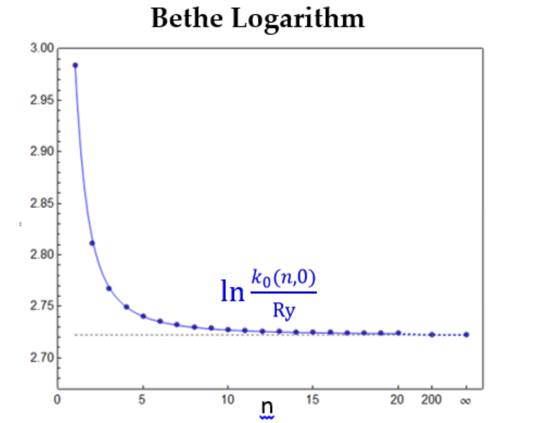
where $\ln k_0(n,l)$ is the Bethe Logarithm, which has been tabulated (Jentschura and Mohr, 2005) for the commonly used values of n and l.

n	$\ln \frac{k_0(n,0)}{\text{Ry}}$	$\ln \frac{k_0(n,1)}{\text{Ry}}$
1	2.984129	---
2	2.811770	-0.0300167
3	2.767664	-0.0381902
4	2.749812	-0.0419549
20	2.723967	-0.0486082
200	2.722668	-0.0490495
∞	2.722654	-0.0490545

Table 3. Bethe Logarithms. The highlighted values (2S, 2P) are used in the Lamb Shift calculation.

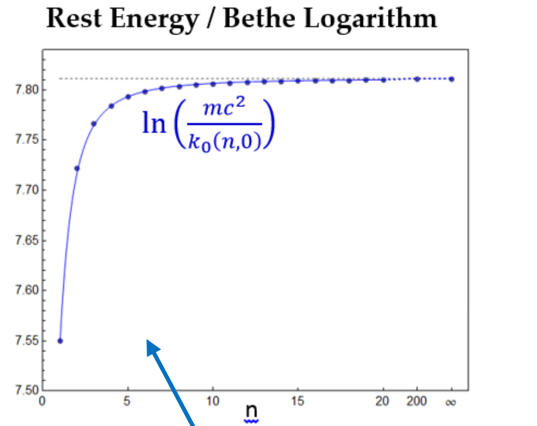
Implications for a Free Electron

Bethe Logarithm



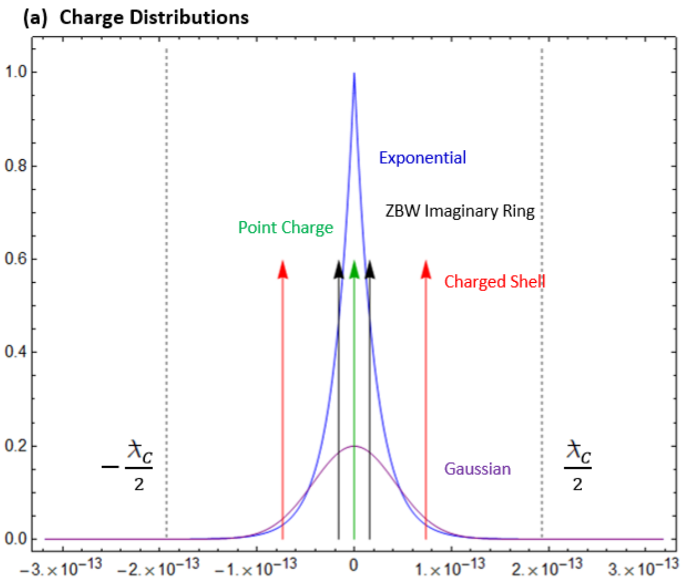
$$\ln \frac{k_0(n,0)}{\mathrm{Ry}} \approx 2.7226543 + \frac{0.5}{n^2} - \frac{0.25}{n^3} + \frac{0.0125}{n^4}$$

Rest Energy / Bethe Logarithm



$$\ln \left(\frac{mc^2}{\mathrm{Ry}}\right) \approx 10.5336344$$

$$\ln \left(\frac{mc^2}{k_0(n,0)}\right) \approx 7.8109801 - \frac{0.5}{n^2} + \frac{0.25}{n^3} - \frac{0.0125}{n^4}$$



$$\Delta E_{<} = mc^2 \frac{4}{3\pi} \frac{(Z\alpha)^4 \alpha}{n^3} \ln \left(\frac{mc^2}{k_0(n,l)}\right)$$

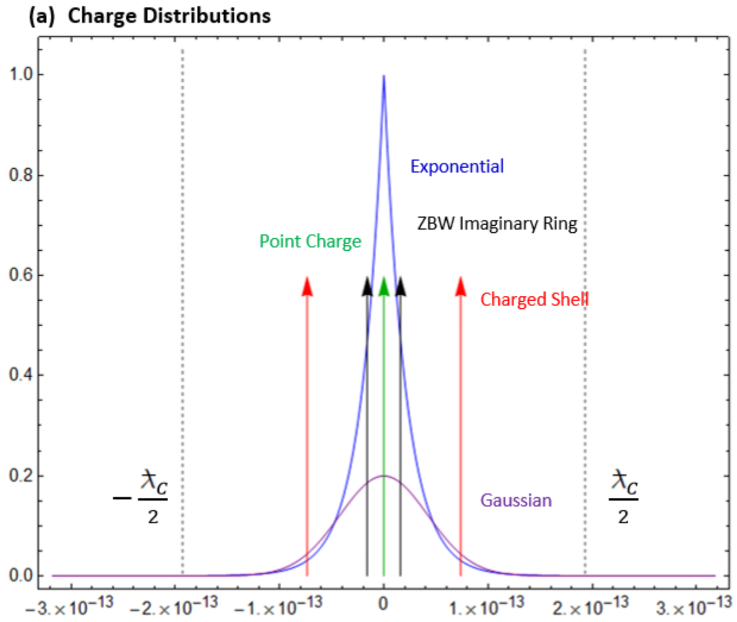
This term only changes by 3.3% from tightly bound to free electron

So the Sub-Compton charge distribution that gave Lamb Shift (bound state) is a good approximation to the charge distribution of a free electron.

?

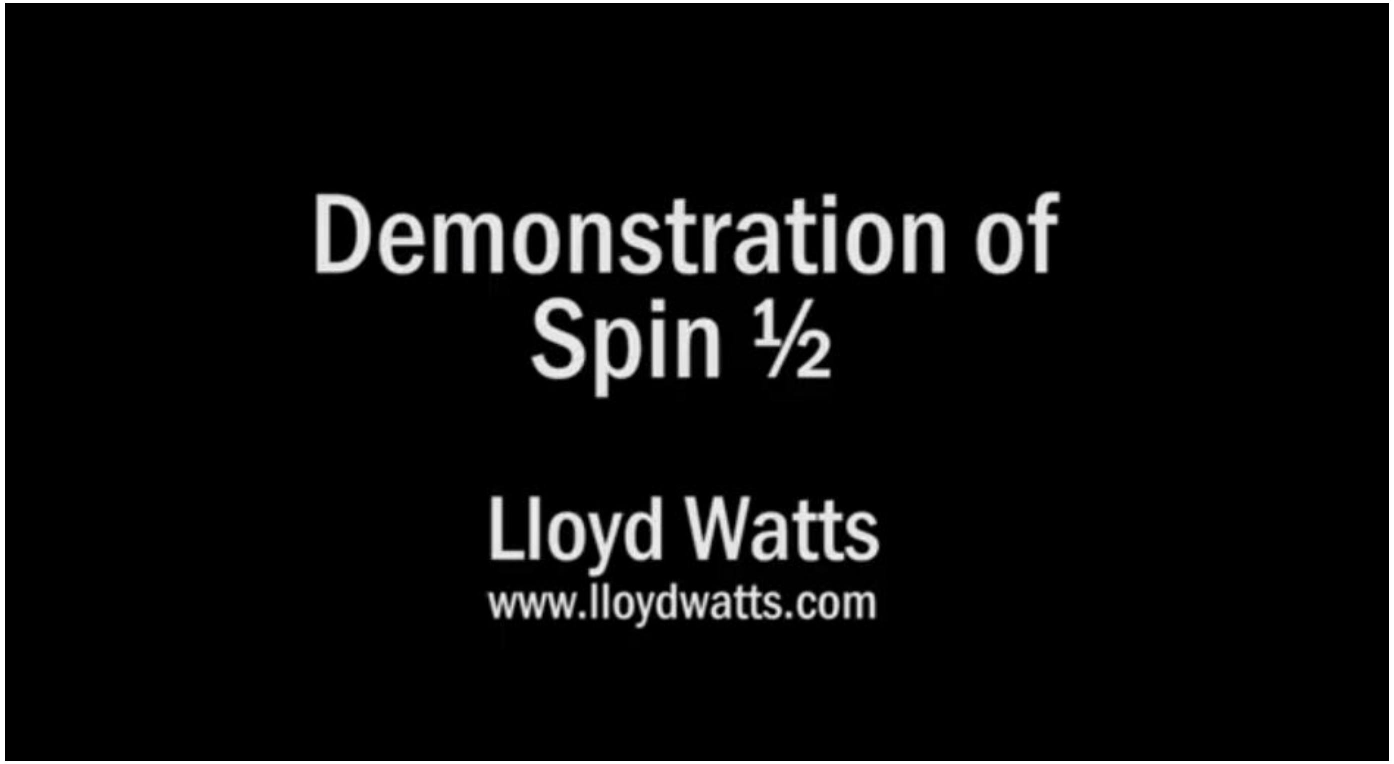
Discussion

All of the candidate charge distributions can be made to agree with Lamb Shift, by correct choice of radius. Is there a higher-order moment that would distinguish between them, or specify the correct shape?



Question for Jentschura and Mohr:
Would the detailed calculation of the Bethe Logarithm allow a determination of the charge distribution (i.e. Fourier Transform to momentum domain, Parseval's Theorem)?

Visualization of Spin ½ Basis Spinors



https://www.youtube.com/watch?v=JFSU9X11wyY

Lamb Shift and Sub-Compton Electron Dynamics: Dirac Hydrogen Wavefunctions without Singularities

Lloyd Watts

October 16, 2015