

# Analytic Evaluation of QED Corrections in One-Electron Ions

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March 27, 2020

# Outline

## 1 Motivation

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- 2 One-Loop QED Corrections

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- 3 Vacuum Polarization Correction

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- 4 Self-Energy Correction to Energy Levels

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# Motivation

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- Theory of Everything

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- Testing Current Fundamental Theories

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- Bound-State Quantum Electrodynamics

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⇒ High-Precision Theory!



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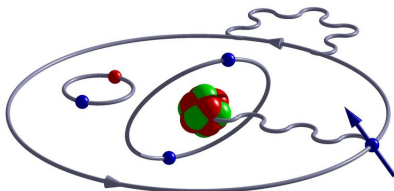
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# Quantum Electrodynamics (QED)

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<sup>1</sup>[https://www.mpi-hd.mpg.de/mpi/fileadmin/bilder/Progress\\_Reports/2017-19/2QuantumDynamics.pdf](https://www.mpi-hd.mpg.de/mpi/fileadmin/bilder/Progress_Reports/2017-19/2QuantumDynamics.pdf)

# Quantum Electrodynamics (QED)



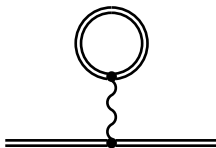
**Figure:** Scheme of the QED contributions to the electronic structure of highly charged ions.<sup>1</sup>

$$\mathcal{L}_{\text{QED}} = \bar{\psi} \left[ \gamma^\mu (i\hbar c \partial_\mu - eA_\mu) - m_e c^2 \right] \psi - \frac{1}{16\pi} F_{\mu\nu} F^{\mu\nu}. \quad (1)$$

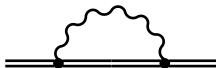
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# One-Loop Energy Corrections

Vacuum Polarization:



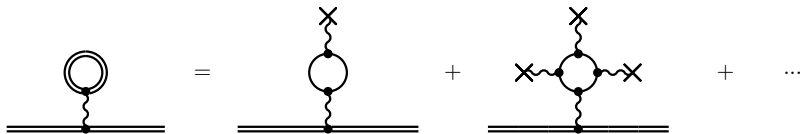
Self-Energy Correction:



# Vacuum Polarization

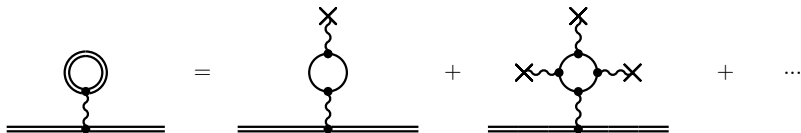
# Vacuum Polarization

Vacuum Polarization:



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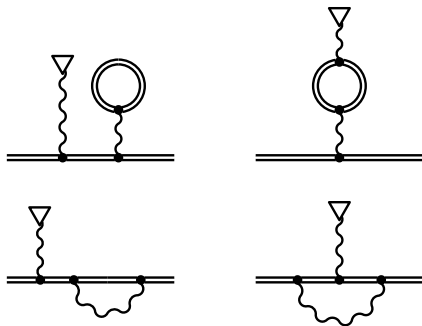
Modification of the Photon Propagator:

$$\begin{aligned}
 iD'_{\mu\nu}(k) &= \text{wavy line} + \text{wavy line with vacuum polarization loop} \\
 &= iD_{\mu\nu}(k) + iD_{\mu\lambda}(k) \frac{i\Pi^{\lambda\sigma}(k)}{4\pi} iD_{\sigma\nu}(k)
 \end{aligned}$$

# One-Loop $g$ Factor Corrections



# One-Loop $g$ Factor Corrections



**Figure:** Feynman diagrams representing the first-order radiative corrections to the  $g$  factor of the bound electron.

## $g$ Factor

The  $g$  Factor is given by [18]:

$$g = -\frac{\kappa}{2j(j+1)} \left( 1 - 2\kappa \frac{\partial E_{n\kappa}}{\partial m_e} \right), \quad (2)$$

if the potential  $V(r)$  does not depend on the electron mass  $m_e$ .

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Small Perturbation of the potential  $\delta V(r)$  leads to

$$\Delta g = -\frac{\kappa^2}{j(j+1)m_e} \left\langle r \frac{\partial \delta V(r)}{\partial r} \right\rangle. \quad (3)$$

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## Leptonic Vacuum Polarization

Leptonic Uehling Potential [9]:

$$\delta V(r) = \frac{\alpha}{\pi} \int_0^1 dv \frac{v^2 (1 - v^2/3)}{1 - v^2} \left( -\frac{Z\alpha}{r} e^{-2m_l r / \sqrt{1-v^2}} \right), \quad (4)$$

where  $m_l$  is the mass of the virtual particle in the fermionic loop.

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Energy Shift of the 1s State:

$$\Delta E_{1s}^{\text{lept. VP}} = \langle \delta V(r) \rangle_{1s} = \int_0^\infty dr (G_{1s}^2(r) + F_{1s}^2(r)) \delta V(r). \quad (5)$$

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$g$  Factor Shift of the 1s State:

$$\Delta g_{1s}^{\text{lept. VP}} = -\frac{4}{3m_e} \left\langle r \frac{\partial \delta V(r)}{\partial r} \right\rangle_{1s}. \quad (6)$$

### 4.1. Energy Shift

We now perform the calculations for the energy shift of the 1s state in hydrogen-like atoms due to the leptonic Uehling potential. When  $|\psi_{1s}\rangle$  denotes the bound electron wave function of the ground state in a point-like Coulomb potential, the energy shift in first-order perturbation theory is given by:

$$\begin{aligned} \Delta E_{1s}^{\text{VP}} &= \langle \psi_{1s} | \delta V(r) | \psi_{1s} \rangle = \int_0^\infty dr (G^2(r) + F^2(r)) \delta V(r) \\ &= \frac{2\lambda}{\Gamma(2\gamma+1)} \int_0^\infty dr (2\lambda r)^{2\gamma} e^{-2\lambda r} \left( -\frac{Z\alpha^2}{4r} \int_0^1 dt \frac{v^2 (1-v^2/3)}{1-v^2} e^{-2m_e r/\sqrt{1-v^2}} \right) \\ &= -\frac{2\lambda Z\alpha^2}{\Gamma(2\gamma+1)\pi} \int_0^1 dt \frac{v^2 (1-v^2/3)}{1-v^2} \int_0^\infty dr \frac{(2\lambda r)^{2\gamma} e^{-2\lambda r}}{r} \left( \lambda + \frac{m_e}{\sqrt{1-v^2}} \right). \end{aligned} \quad (4.4)$$

Now, substitute  $u = r^{2\gamma}$ ,  $du = 2\gamma r^{2\gamma-1} dr$ .

and then  $t = \left[ 2 \left( \lambda + \frac{m_e}{\sqrt{1-v^2}} \right) \right]^{2\gamma} u$ ,  $dt = \left[ 2 \left( \lambda + \frac{m_e}{\sqrt{1-v^2}} \right) \right]^{2\gamma} du$ :

$$\begin{aligned} \Delta E_{1s}^{\text{VP}} &= -\frac{2\lambda Z\alpha^2}{\Gamma(2\gamma+1)\pi} \int_0^1 dt \frac{v^2 (1-v^2/3)}{1-v^2} \int_0^\infty \frac{du}{2\gamma} (2\lambda)^{2\gamma} e^{-2\lambda^{1/(2\gamma)} \left( \lambda + \frac{m_e}{\sqrt{1-v^2}} \right) u} \\ &= -\frac{2\lambda Z\alpha^2}{\Gamma(2\gamma+1)\pi} \int_0^1 dt \frac{v^2 (1-v^2/3)}{1-v^2} \frac{(2\lambda)^{2\gamma}}{2\gamma \left[ 2 \left( \lambda + \frac{m_e}{\sqrt{1-v^2}} \right) \right]^{2\gamma}} \int_0^\infty dt e^{-t^{1/(2\gamma)}} \\ &= -\frac{Z\alpha^2 \lambda^{2\gamma+1}}{\gamma\pi} \int_0^1 dt \frac{v^2 (1-v^2/3) (1-v^2)^{-\gamma-1}}{\left[ \lambda \sqrt{1-v^2} + m_e \right]^{2\gamma}} \\ &= -\frac{Z\alpha^2 (sZ\alpha)^2 \lambda}{\gamma\pi} \int_0^1 dt \frac{v^2 (1-v^2/3) (1-v^2)^{-\gamma-1}}{\left[ 1 + sZ\alpha \sqrt{1-v^2} \right]^{2\gamma}}, \end{aligned} \quad (4.5)$$

where we used the relation  $\Gamma(x+1) = x\Gamma(x)$  and that  $\lambda/m_e = sZ\alpha$ , where  $s = m_e/m_l$  is the ratio of the electron and the loop particle masses.

This integral can now be solved analytically with the base integral given in [28]:

$$\begin{aligned} I_{abc} &= \int_0^1 dy \frac{(1-y)^{c-1/2}}{y^{b-1}} \left( \frac{sZ\alpha y}{1+sZ\alpha y} \right)^{-c-2a} \\ &= \frac{1}{2} (sZ\alpha)^{-c-2a} B \left( a + \frac{1}{2}, 1 - \frac{b-c}{2} - c \right) \\ &\quad \times {}_3F_2 \left( \frac{c}{2} - c, \frac{c+1}{2} - c, 1 - \frac{b-c}{2} - c; \frac{1}{2}, a + \frac{3-b+c}{2} - c; (sZ\alpha)^2 \right) \\ &\quad - \frac{c-2c}{2} (sZ\alpha)^{c+1-2a} B \left( a + \frac{1}{2}, \frac{3-b+c}{2} - c \right) \\ &\quad \times {}_3F_2 \left( \frac{c}{2} + 1 - c, \frac{c+1}{2} - c, \frac{3-b+c}{2} - c; \frac{3}{2}, a + 2 - \frac{b-c}{2} - c; (sZ\alpha)^2 \right). \end{aligned} \quad (4.6)$$

Here,  $\epsilon = 1 - \gamma$ , and  $B(x, y)$  is the beta function defined in Appendix A.4. Performing the substitution  $y = \sqrt{1-v^2}$ ,  $dy = \frac{v dv}{\sqrt{1-v^2}}$ , one obtains finally:

$$\begin{aligned} \Delta E_{1s}^{\text{VP}} &= -\frac{Z\alpha^2 (sZ\alpha)^2 \lambda}{\gamma\pi} \left[ \int_0^1 \frac{y dy}{\sqrt{1-y^2}} \frac{(1-y^2)^{\gamma-3/2}}{1+sZ\alpha y^{2\gamma}} - \frac{1}{3} \int_0^1 \frac{y dy}{\sqrt{1-y^2}} \frac{(1-y^2)^{\gamma-2}}{1+sZ\alpha y^{2\gamma}} \right] \\ &= -\frac{Z\alpha^2 \lambda}{\gamma\pi} \left[ \int_0^1 \frac{dy}{y} \frac{(1-y^2)^{\frac{3}{2}}}{1+sZ\alpha y^{2\gamma}} \left( \frac{sZ\alpha y}{1+sZ\alpha y} \right)^{2\gamma} - \int_0^1 \frac{dy}{y} \frac{(1-y^2)^{\frac{5}{2}}}{1+sZ\alpha y^{2\gamma}} \left( \frac{sZ\alpha y}{1+sZ\alpha y} \right)^{2\gamma} \right] \\ &= -\frac{Z\alpha^2 \lambda}{\gamma\pi} \left[ I_{222} - \frac{1}{3} I_{222} \right]. \end{aligned} \quad (4.7)$$

This result was already derived in [27] and reference therein. The difference is that in [27], the result was derived for the electron as loop-particle and electrons or muons as bound particles. Here, we considered the electron as bound particle and arbitrary leptons as loop-particles.

To investigate this all-order in  $Z\alpha$  result, we may expand (4.7) in a series for small  $Z\alpha$  to get a simple and handy formula for the correction due to the leptonic Uehling potential. Using the computer algebra software *Mathematica* [18], we find for the leading order Taylor expansion:

$$\begin{aligned} \Delta E_{1s}^{\text{VP}} &= \frac{\alpha m_e}{\pi} \left[ -\frac{4s^2(Z\alpha)^4}{15} + \frac{5\pi s^3(Z\alpha)^5}{48} \right. \\ &\quad + \left( \frac{4s^2}{15} \ln(2sZ\alpha) - \frac{107s^2}{225} - \frac{12s^4}{35} \right) (Z\alpha)^6 \\ &\quad \left. + \left( -\frac{5\pi s^3}{48} \ln \left( \frac{sZ\alpha}{2} \right) - \frac{17\pi s^3}{576} + \frac{7\pi s^5}{64} \right) (Z\alpha)^7 + \mathcal{O}(Z\alpha)^8 \right]. \end{aligned} \quad (4.8)$$

Therefore, the energy shift correction for leptonic vacuum polarization is of the leading order  $(Z\alpha)^4$ . The first term of expression (4.8) coincides with the result of the simplest approximation, namely, using nonrelativistic wave functions and the low-momentum approximation of the polarization function [13, 16, 24]. Since this leads to a Dirac delta function, we will call it the  $\delta$ -potential approximation.

With formula (4.7), one can calculate the energy shift contribution for any leptonic vacuum loop.<sup>2</sup> As equation (4.7) or (4.8) show, the heavier the loop particle is, the smaller is the measurable effect. After the  $e^-e^+$ -loop, the next important contribution is due to the  $\mu^- \mu^+$ -loop, also called muonic vacuum polarization, where a muon and anti-muon pair is produced in the loop. The effect of muonic vacuum polarization is around  $s^2 \approx 1/207^2 \approx 2 \cdot 10^{-5}$  times smaller than that of the electronic vacuum polarization.

Figure 4.1 shows the absolute value of the muonic vacuum polarization contribution to the energy shift for different charge numbers  $Z$ , calculated with the exact formula (4.7) and its approximation (4.8) up to 5th order. It should be mentioned that the Uehling potential is attractive and results in a stronger binding. Thus, the corresponding energy shift is negative. The correction for ions with charge numbers  $Z \leq 8$  is so small that its value is not visible in this diagram.

<sup>2</sup>As mentioned in [28], this formula can be applied to regular, electronic atoms or ions considered in this work, or to muonic atoms by replacing the electron mass  $m_e$  with the muon mass  $m_\mu$ .



# Leptonic Vacuum Polarization

Energy Shift for a point-like Nucleus:

$$\Delta E_{1s}^{\text{lept. VP}} = -\frac{Z\alpha^2\lambda}{\gamma\pi} \left[ I_{122} - \frac{1}{3} I_{222} \right]. \quad (7)$$

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$g$  Factor Shift for a point-like Nucleus:

$$\Delta g_{1s}^{\text{lept. VP}} = -\frac{8\alpha(Z\alpha)}{3\pi s} \left[ I_{133} - \frac{1}{3} I_{233} + \frac{Z\alpha s}{2\gamma} \left( I_{122} - \frac{1}{3} I_{222} \right) \right]. \quad (8)$$

# Hadronic Vacuum Polarization

## Hadronic Vacuum Polarization

Real Part of the Hadronic Polarization Function [4]:

$$\text{Re} [\Pi_{\text{had}}(q^2)] = A_i + B_i \ln(1 + C_i q^2), \quad (9)$$

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$$\text{Re} [\Pi_{\text{had}}(q^2)] = A_i + B_i \ln(1 + C_i q^2), \quad (9)$$

The parameters are given by

| i | Region        | Range [GeV]     | $A_i$     | $B_i$     | $C_i$ [GeV <sup>-2</sup> ] |
|---|---------------|-----------------|-----------|-----------|----------------------------|
| 1 | 0 - $k_1$     | 0.0 - 0.7       | 0.0       | 0.0023092 | 3.9925370                  |
| 2 | $k_1$ - $k_2$ | 0.7 - 2.0       | 0.0       | 0.0022333 | 4.2191779                  |
| 3 | $k_2$ - $k_3$ | 2.0 - 4.0       | 0.0       | 0.0024402 | 3.2496684                  |
| 4 | $k_3$ - $k_4$ | 4.0 - 10.0      | 0.0       | 0.0027340 | 2.0995092                  |
| 5 | $k_4$ - $k_5$ | 10.0 - $m_Z$    | 0.0010485 | 0.0029431 | 1.0                        |
| 6 | $k_5$ - $k_6$ | $m_Z$ - $10^4$  | 0.0012234 | 0.0029237 | 1.0                        |
| 7 | $k_5$ - $k_6$ | $10^4$ - $10^5$ | 0.0016894 | 0.0028984 | 1.0                        |

## Hadronic Uehling Potential

Numerical Hadronic Uehling Potential for a point-like Nucleus:

$$\delta V_{\text{numerical}}^{\text{had. VP}}(r) = -\frac{2Z\alpha}{\pi} \sum_{k=1}^7 \int_{k_{i-1}}^{k_i} dq \frac{\sin(qr)}{qr} [A_i + B_i \ln(1 + C_i q^2)]. \quad (10)$$

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Analytical Hadronic Uehling Potential for a point-like Nucleus:

$$\begin{aligned} \delta V_{\text{analytical}}^{\text{had. VP}}(r) &= -\frac{2Z\alpha}{\pi} \int_0^\infty dq \frac{\sin(qr)}{qr} [A_1 + B_1 \ln(1 + C_1 q^2)] \\ &= -\frac{2Z\alpha}{r} B_1 E_1 \left( \frac{r}{\sqrt{C_1}} \right). \end{aligned} \quad (11)$$

# Hadronic Uehling Potential

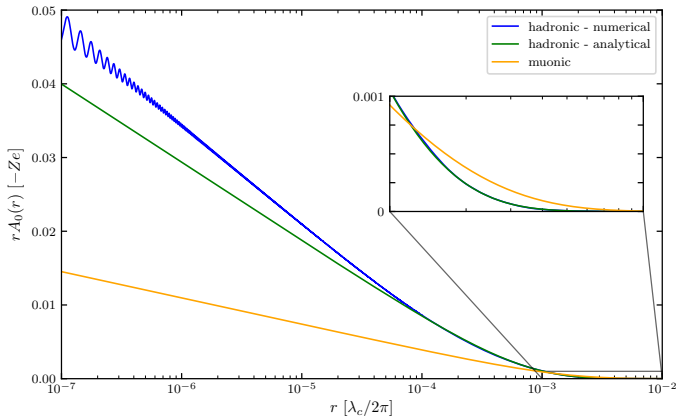


Figure: Comparison of leptonic and hadronic Uehling potential.



# Hadronic Energy Shift

## Hadronic Energy Shift

Energy Shift of the 1s State for a point-like Nucleus:

$$\Delta E_{1s}^{\text{had. VP}} = -\frac{Z\alpha\lambda(2\lambda\sqrt{C_1})^{2\gamma} B_1}{\gamma^2} {}_2F_1\left(2\gamma, 2\gamma; 1 + 2\gamma; -2\lambda\sqrt{C_1}\right). \quad (12)$$

## Hadronic Energy Shift

Energy Shift of the 1s State for a point-like Nucleus:

$$\Delta E_{1s}^{\text{had. VP}} = -\frac{Z\alpha\lambda(2\lambda\sqrt{C_1})^{2\gamma} B_1}{\gamma^2} {}_2F_1\left(2\gamma, 2\gamma; 1 + 2\gamma; -2\lambda\sqrt{C_1}\right). \quad (12)$$

$Z\alpha$  Expansion:

$$\begin{aligned} \Delta E_{1s}^{\text{had. VP}} \approx & -4B_1 C_1 m_e^3 (Z\alpha)^4 + \frac{32B_1 C_1^{3/2} m_e^4 (Z\alpha)^5}{3} \\ & - 4B_1 C_1 m_e^3 (Z\alpha)^6 \left[ 1 + 6C_1 m_e^2 - \ln(2Z\alpha\sqrt{C_1} m_e) \right]. \end{aligned} \quad (13)$$

## Hadronic Energy Shift

| $Z$ | $\Delta E_{\text{analytical}}^{\text{point}}$ [eV] | $\Delta E_{\text{numerical}}^{\text{point}}$ [eV] | $\Delta E_{\text{exact}}^{\text{finite size}}$ [eV] |
|-----|--|---|---|
| 1   | $-1.3963 \cdot 10^{-11}$                           | $-1.39(33) \cdot 10^{-11}$                        | $-1.391(4) \cdot 10^{-11}$                          |
| 14  | $-5.9178 \cdot 10^{-7}$                            | $-5.90(18) \cdot 10^{-7}$                         | $-5.756(1) \cdot 10^{-7}$                           |
| 20  | $-2.7133 \cdot 10^{-6}$                            | $-2.71(5) \cdot 10^{-6}$                          | $-2.5596(3) \cdot 10^{-6}$                          |
| 70  | $-3.1090 \cdot 10^{-3}$                            | $-3.109(4) \cdot 10^{-3}$                         | $-1.248(1) \cdot 10^{-3}$                           |
| 82  | $-1.4128 \cdot 10^{-2}$                            | $-1.413(1) \cdot 10^{-2}$                         | $-3.693(4) \cdot 10^{-3}$                           |

Table: Energy shifts for hadronic VP.

# Hadronic $g$ Factor Shift

## Hadronic $g$ Factor Shift

$g$  Factor Shift of the 1s State for a point-like Nucleus:

$$\Delta g_{1s}^{\text{had. VP}} = -\frac{8B_1(Z\alpha)^2(2\lambda\sqrt{C_1})^{2\gamma}}{3\gamma(1+2\lambda\sqrt{C_1})^{2\gamma}} + \frac{4}{3m_e}\Delta E_{\text{approx.}} \quad (14)$$

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$Z\alpha$  Expansion:

$$\begin{aligned} \Delta g_{1s}^{\text{had. VP}} \approx & -16B_1C_1m_e^2(Z\alpha)^4 + \frac{512B_1C_1^{3/2}m_e^3(Z\alpha)^5}{9} \\ & - \frac{16B_1C_1m_e^2(Z\alpha)^6}{3} \left[ 2 + 30C_1m_e^2 - 3\ln(2m_eZ\alpha\sqrt{C_1}) \right]. \end{aligned} \quad (15)$$

## Hadronic $g$ Factor Shift

| $Z$ | $\Delta g_{\text{analytical}}^{\text{point}}$ | $\Delta g_{\text{numerical}}^{\text{point}}$ | $\Delta g_{\text{approx}}^{\text{finite size}}$ |
|-----|---|--|---|
| 1   | $-1.0929 \cdot 10^{-16}$                      | $-1.09(9) \cdot 10^{-16}$                    | $-1.09(2) \cdot 10^{-16}$                       |
| 14  | $-4.6157 \cdot 10^{-12}$                      | $-4.61(5) \cdot 10^{-12}$                    | $-4.49(1) \cdot 10^{-12}$                       |
| 20  | $-2.1085 \cdot 10^{-11}$                      | $-2.11(2) \cdot 10^{-11}$                    | $-1.99(1) \cdot 10^{-11}$                       |
| 70  | $-2.2051 \cdot 10^{-8}$                       | $-2.205(1) \cdot 10^{-8}$                    | $-8.86(1) \cdot 10^{-9}$                        |
| 82  | $-9.5886 \cdot 10^{-8}$                       | $-9.589(3) \cdot 10^{-8}$                    | $-2.51(1) \cdot 10^{-8}$                        |

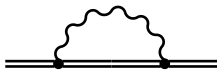
Table:  $g$  factor shifts for hadronic VP.



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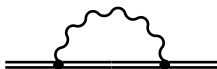
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## Self-Energy Correction



$$\Delta E^{\text{SE}} = -ie^2 \int \frac{d^4 k}{(2\pi)^4} \frac{1}{k^2} \left\langle \psi \left| \gamma^\mu \frac{1}{\not{p} - \not{k} - m_e - \gamma^0 V} \gamma_\mu \right| \psi \right\rangle. \quad (16)$$

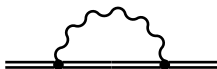
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⇒ Approximation!

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This Regularization Technique yields the well-known Result [9]

$$\Delta E_{1s}^{\text{SE}} = \frac{4\alpha}{3\pi} (Z\alpha)^4 m_e \left[ \frac{5}{6} - 2 \ln(Z\alpha) - \ln k_0 \right], \quad (17)$$

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where the Bethe logarithm  $\ln k_0$  is defined as

$$\frac{(Z\alpha)^4 m_e}{n^3} \ln k_0 = \frac{1}{2m_e^2} \left\langle \mathbf{p} (H - E) \ln \left[ \frac{2(H - E)}{m_e(Z\alpha)^2} \right] \mathbf{p} \right\rangle. \quad (18)$$



## Bethe Logarithm

Integral representation of the Bethe logarithm [13]:

$$\ln k_0(n) = -\frac{3}{4} PV \int_0^1 dt \frac{1}{t^3} \left( \frac{t^2 - 1}{nt^2} P_{nd}(t) + \frac{2}{3n} - \frac{8t^2}{3} \right) - 2 \ln(n), \quad (19)$$

$PV$  denotes the principal value and  $P_{nd}(t)$  is the non-relativistic dipol matrix element:

$$P_{nd} = \frac{1}{3m_e} \left\langle \phi_{nlm} \left| \mathbf{p} \frac{1}{H - (E - \omega)} \mathbf{p} \right| \phi_{nlm} \right\rangle. \quad (20)$$

# Outline

- 1 Motivation
- 2 One-Loop QED Corrections
- 3 Vacuum Polarization Correction
  - Leptonic
  - Hadronic
- 4 Self-Energy Correction to Energy Levels
- 5 Conclusion and Outlook

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⇒ Plenty of Room for Analytical Work!



Thank you and stay healthy!



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