

NRQED

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Introduction

1 Hydrogen Wavefunction Divergence Near Origin in Dirac Equation and Schrödinger Equation

1.1 The Dirac part

The Dirac Hydrogen Equation is

$$(\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m - \frac{Z\alpha}{r})\Psi = E\Psi \quad (1)$$

For the bound state, the wavefunction¹ is [Darwin(1928), Gordon(1928), Bethe *et al.*(2008)Bethe, Salpeter, and Physics]

$$\Psi_{1, \frac{1}{2}, \frac{1}{2}}^+ = \begin{bmatrix} \frac{ic\sqrt{m+E}\rho^\gamma e^{-\frac{\rho}{2}}}{r} \sqrt{\frac{1}{4\pi}} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ -\frac{c\sqrt{m-E}\rho^\gamma e^{-\frac{\rho}{2}}}{r} \sqrt{\frac{1}{4\pi}} \begin{bmatrix} \cos \theta \\ \sin \theta e^{i\phi} \end{bmatrix} \end{bmatrix} \quad (2)$$

$$\Psi_{1, \frac{1}{2}, -\frac{1}{2}}^+ = \begin{bmatrix} \frac{ic\sqrt{m+E}\rho^\gamma e^{-\frac{\rho}{2}}}{r} \sqrt{\frac{1}{4\pi}} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ -\frac{c\sqrt{m-E}\rho^\gamma e^{-\frac{\rho}{2}}}{r} \sqrt{\frac{1}{4\pi}} \begin{bmatrix} \sin \theta e^{i\phi} \\ \cos \theta \end{bmatrix} \end{bmatrix} \quad (3)$$

where

$$E = m\gamma, \quad \rho = 2\lambda r, \quad \lambda = mZ\alpha, \quad \gamma = \sqrt{1 - Z^2\alpha^2}, \quad c = \sqrt{\frac{Z\alpha}{\Gamma(2\gamma + 1)}} \quad (4)$$

c is the normalization factor for $\int d^3r |\Psi|^2 = 1$.

Only keeping the upper component ψ_u , we need to normalize it again so that $\int d^3r \psi_u^2 \approx 1$. We get an extra normalization factor

$$1 - \frac{\lambda^2}{8m^2} + \frac{2\gamma\lambda}{4m^2r} - \frac{\gamma^2 - \gamma}{8m^2r^2}$$

For convenience, define

$$\psi'_u = \frac{\psi_u}{2(mZ\alpha)^{\frac{3}{2}}} \quad (5)$$

Now Ψ' is dimensionless and expand it in α , we get the logarithmic divergence comes from a term

$$R(r) \sim -\frac{(Z\alpha)^2}{2} \log(2mZ\alpha r) \quad (6)$$

the m in log could be interpreted as a subtraction point μ .

¹This wavefunction checks out with Bethe's, except for an extra i .

1.2 The Schrödinger part

The Hamiltonian is

$$H = H_0 + H_{int} \quad (7)$$

$$H_0 = -\frac{\nabla^2}{2m} - \frac{Z\alpha}{r}, \quad H_{int} = \frac{\nabla^4}{8m^3} - \frac{1}{8m^2} \nabla^2 \frac{Z\alpha}{r} + \frac{1}{4m^2} \frac{Z\alpha}{r^3} \boldsymbol{\sigma} \cdot \mathbf{L} \quad (8)$$

The first term of H_{int} is the relativistic kinematic v^2 correction, the second one is the Darwin term. For S-wave state, it's obvious that the third term, spin-orbital interaction has no contribution.

The H_0 gives the radial wave functions as follows

$$R_{n0} = \frac{2(mZ\alpha)^{\frac{3}{2}}}{n^{\frac{3}{2}}} e^{-\frac{mZ\alpha}{n}r} F(1-n, 2, \frac{2mZ\alpha r}{n}), \quad E_n = -\frac{Z^2\alpha^2 m}{2n^2} \quad (9)$$

$$R_{\kappa 0} = \sqrt{\frac{2}{\pi}} (mZ\alpha)^{\frac{3}{2}} \kappa e^{\frac{\pi}{2\kappa}} |\Gamma(1 - \frac{i}{\kappa})| e^{-imZ\alpha\kappa r} F(1 + \frac{i}{\kappa}, 2, 2imZ\alpha\kappa r), \quad E_{\kappa} = \frac{mZ^2\alpha^2\kappa^2}{2} \quad (10)$$

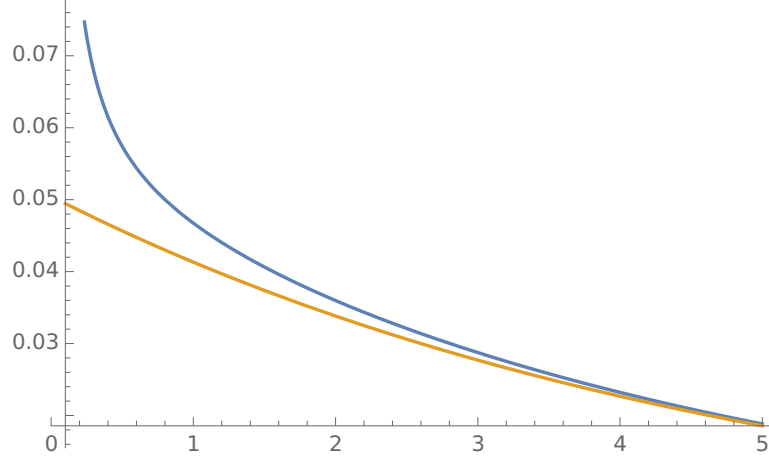


Figure 1: Comparison between Dirac wavefunction and Schrödinger wavefunction near origin.

The NLO correction of the bound state wave function is

$$\sum_{n \neq 1} a_{n1} \phi_{n00} + \int d\kappa a_{\kappa 1} \phi_{\kappa 00} \quad (11)$$

with

$$a_{n1} = \frac{\langle \phi_{n00} | H_{int} | \phi_{100} \rangle}{E_1 - E_n} \quad (12)$$

The relativistic correction is the same with Klein-Gordon equation

$$R^{(1)}(0)_{kin} = \int^{\Lambda} d\kappa (Z\alpha)^2 \left(\frac{1}{\pi} + \frac{1}{\kappa} \right) \quad (13)$$

$$\sim (\alpha Z)^2 \left(\frac{\Lambda}{\pi} + \log \Lambda \right) \quad (14)$$

The UV divergent part of Darwin term is

$$R^{(1)}(0)_D = \int^{\Lambda} d\kappa \left(-\frac{\alpha^2 e^{\frac{\pi}{2\kappa}} \kappa Z^2 |\Gamma(\frac{-i+\kappa}{\kappa})|}{\kappa^2 + 1} \right) \psi_{\kappa 00} \quad (15)$$

$$\sim -\frac{\alpha^2 \Lambda Z^2}{2\pi} - \frac{1}{2} \alpha^2 Z^2 \log(\Lambda) \quad (16)$$

Now collect all the results we get as follow.

The Dirac wave function's origin UV divergence is

$$Dirac \text{ UV} : \frac{Z^2 \alpha^2}{16m^2 r^2} + \frac{Z\alpha}{2mr} - \frac{(Z\alpha)^2}{2} \log(mr) \quad (17)$$

The purterbative Schrödinger wave function's origin UV divergence, with a κ cutoff Λ , is

$$Kin \text{ UV} : (\alpha Z)^2 \left(\frac{\Lambda}{\pi} + \log \Lambda \right) \quad (18)$$

$$Darwin \text{ UV} : -\frac{\alpha^2 \Lambda Z^2}{2\pi} - \frac{1}{2} \alpha^2 Z^2 \log(\Lambda) \quad (19)$$

2 Non-relativistic QED (NRQED) Matching

2.1 Feynman Rules

2.1.1 QED

Lagrangian

$$\mathcal{L}_{QED} = \bar{\psi}(i\not{D} - m)\psi + \Phi_v^* i v \cdot D \Phi_v \quad (20)$$

with

$$D_\mu \phi = \partial_\mu \phi + ie A_\mu \phi$$

and

$$D_\mu \Phi_v = \partial_\mu \Phi - iZe A_\mu \Phi_v$$

But note that no \mathbf{A} can appear in actual calculation because here only static scalar potential exists. And the Feynman rules are standard QED and HQET Feynman rules except that photons only appear as zero component of Coulomb gauge photon to describe Coulomb potential exchange.

Here v satisfies on-shell condition $v^2 = 1$ and the k with it stands for the offshellness of the propagating momentum.

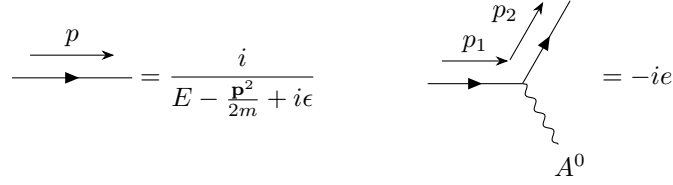
2.1.2 NRQED

Using the Foldy-Wouthuysen transformation, we can have the Lagrangian

$$\mathcal{L}_{NRQED} = \bar{\psi}_e \left(iD_0 + \frac{\mathbf{D}^2}{2m} \right) \psi_e + \delta \mathcal{L} + \Phi_v^* i v \cdot D \Phi_v \quad (21)$$

with the same notation above. Here $\mathbf{D} = \nabla - ie\mathbf{A}$.

Feynman rules are also the same except for the scalar electron side which becomes



The diagram shows two Feynman rules. The first rule is for a scalar electron propagator: a horizontal line with an arrow pointing right, labeled with momentum p , is equal to the expression $\frac{i}{E - \frac{\mathbf{p}^2}{2m} + i\epsilon}$. The second rule is for a photon vertex: a horizontal line with an arrow pointing right, labeled with momentum p_1 , meets a vertical wavy line labeled A^0 . From this vertex, another line goes up and to the right, labeled with momentum p_2 . This vertex is equal to $-ie$.

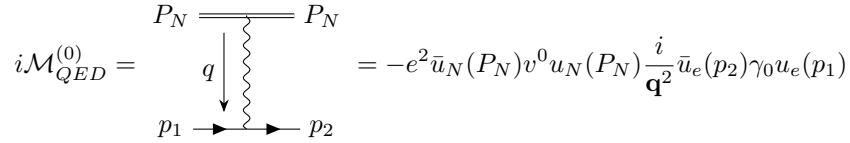
We can ignore all interacting terms involving \mathbf{A} .

Another way to achieve it is to use the transform rules of heavy quark effective theory (HQET) and change the power counting.

2.2 LO Matching

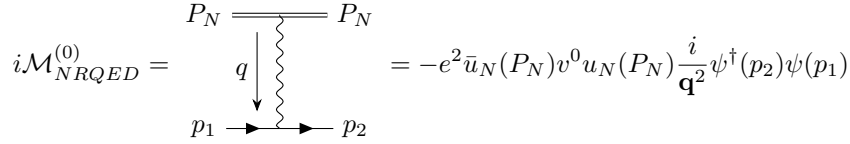
2.2.1 QED

In tree level²



The diagram shows a tree-level matching calculation. On the left, a heavy particle line (double line) with momentum P_N and a scalar electron line (single line with arrow) with momentum p_1 meet at a vertex. A wavy line labeled q connects this vertex to another vertex where the heavy particle line continues with momentum P_N and the scalar electron line continues with momentum p_2 . The expression for this is $i\mathcal{M}_{QED}^{(0)} =$ followed by the diagram, which is equal to $-e^2 \bar{u}_N(P_N) v^0 u_N(P_N) \frac{i}{\mathbf{q}^2} \bar{u}_e(p_2) \gamma_0 u_e(p_1)$.

2.2.2 NRQED



The diagram shows a tree-level matching calculation for NRQED. It is identical to the QED diagram, but the scalar electron line is now a Dirac spinor line (single line with arrow). The expression for this is $i\mathcal{M}_{NRQED}^{(0)} =$ followed by the diagram, which is equal to $-e^2 \bar{u}_N(P_N) v^0 u_N(P_N) \frac{i}{\mathbf{q}^2} \psi^\dagger(p_2) \psi(p_1)$.

Using Dirac representation, the Dirac spinor is

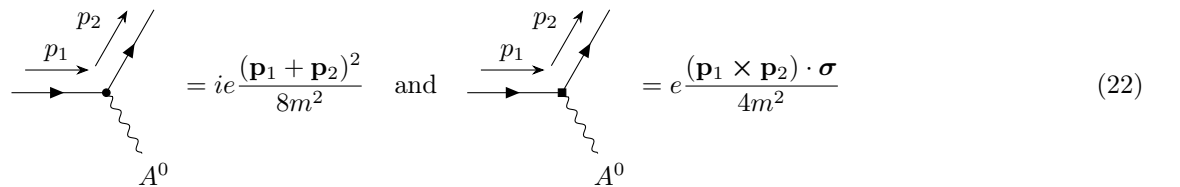
$$u_e(p) = \sqrt{\frac{p^0 + m}{2p^0}} \begin{pmatrix} \psi(p) \\ \frac{\mathbf{p} \cdot \boldsymbol{\sigma}}{p^0 + m} \psi(p) \end{pmatrix}$$

Expand to v^2 order, we have an extra vertex $\frac{\mathbf{p}_1^2 + \mathbf{p}_2^2 - 2\mathbf{p}_1 \cdot \mathbf{p}_2 - 2i(\mathbf{p}_1 \times \mathbf{p}_2) \cdot \boldsymbol{\sigma}}{8m^2}$ which is exactly those terms with denominator $1/8m^2$ in BBL³.

Rather than write down the effective electron-photon vertex up to $\mathcal{O}(v^2)$

$$\left[1 - \frac{(\mathbf{p}_1 + \mathbf{p}_2)^2 - 2i(\mathbf{p}_1 \times \mathbf{p}_2) \cdot \boldsymbol{\sigma}}{8m^2} \right]$$

we can add additional vertexes



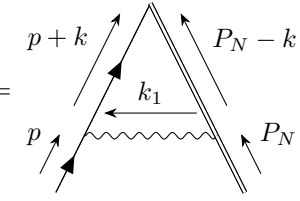
The diagram shows two additional vertexes. The first vertex is a scalar electron line (single line with arrow) with momentum p_1 entering from the left, and a photon line (wavy line) labeled A^0 exiting downwards. A second line enters from the top-left, labeled with momentum p_2 . This vertex is equal to $ie \frac{(\mathbf{p}_1 + \mathbf{p}_2)^2}{8m^2}$. The second vertex is identical, but the incoming line from the top-left is a Dirac spinor line (single line with arrow). This vertex is equal to $e \frac{(\mathbf{p}_1 \times \mathbf{p}_2) \cdot \boldsymbol{\sigma}}{4m^2}$. The entire equation is labeled (22).

²Note that there's no Gamma matrices in the heavy particle side, they can only appear in the QED side.

³Which contains both Darwin and spin-orbital terms

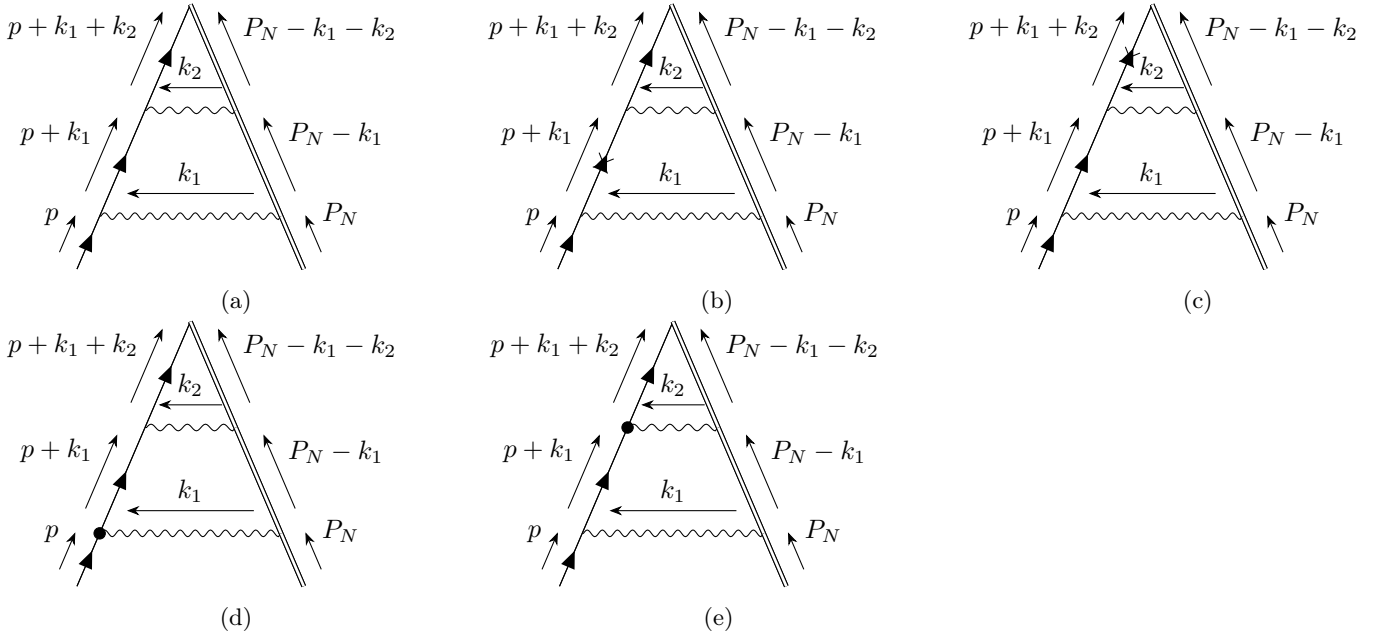
3 Local Operator and Matrix Element of NRQED

3.1 NLO

$$\langle 0 | \psi_e(0) N(0) (-ie\mu^{-\epsilon}) \int d^4 y \bar{\psi}_e \psi_e A^0 (-ie\mu^{-\epsilon}) \int d^4 z \bar{N} N A^0 | eN \rangle =$$


which doesn't have logarithm divergence. We can rigorously prove that so long as there's no dynamic photon, NRQED has no logarithmic divergence at one loop order (at least for this problem we're considering).

3.2 NNLO

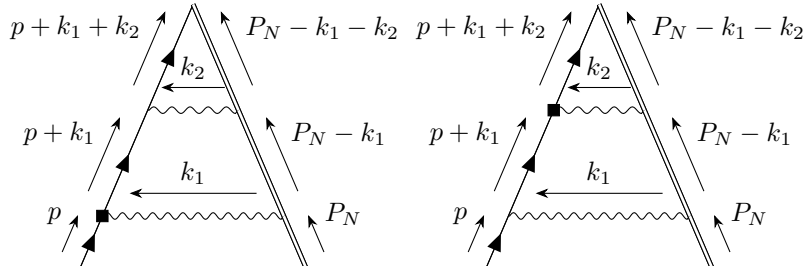


After summing those all together, we get

$$Z^2 \alpha^2 \left(\frac{1}{4(d-3)} - \frac{\log \mu}{2} \right).$$

We can see that the coefficient of $\log \mu$ is exact the same as which of $\log \Lambda$ in the Schrödinger wavefunction with \mathbf{p}^4 relativistic correction and of $\log r$ in Dirac wavefunction.

There're also spin-orbital terms, for example the lowest order appears as the second vertex at (22). By substituting the normal $-ie$ vertex with spin-orbital vertex, we can calculate their contribution order by order. At $Z^2 \alpha^2$ order, there's only two diagrams

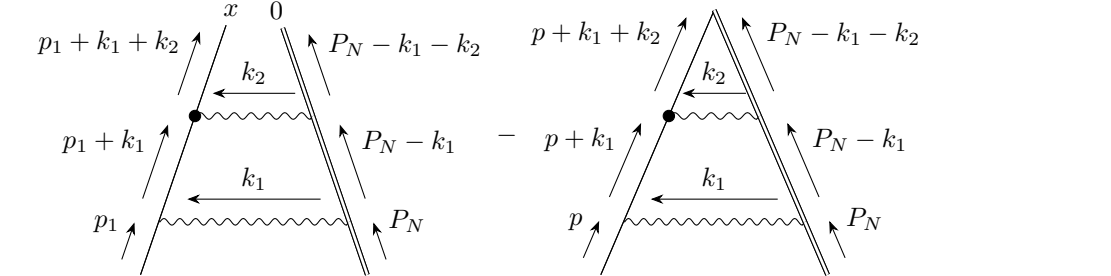


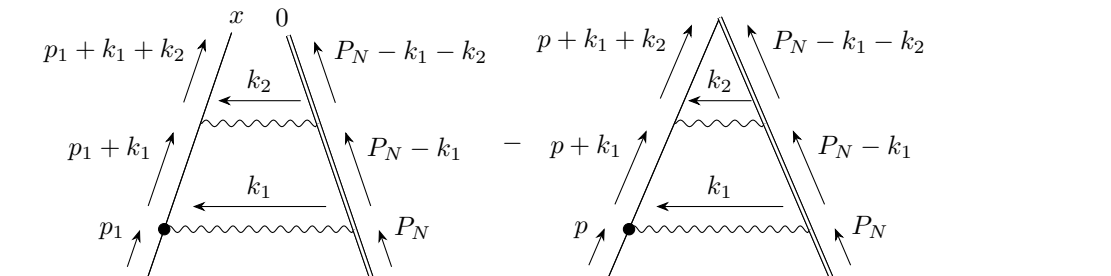
The first one gives $\mathbf{p} \cdot (\boldsymbol{\sigma} \times \mathbf{p})$ and the second one ends up with $\mathbf{k}_1 \cdot (\boldsymbol{\sigma} \times \mathbf{k}_1)$ after integrated the first loop so they're zero.

4 OPE

The relativistic correction part is the same as scalar ones.

The Darwin term gives an additional vertex in (22), and that contains two diagrams



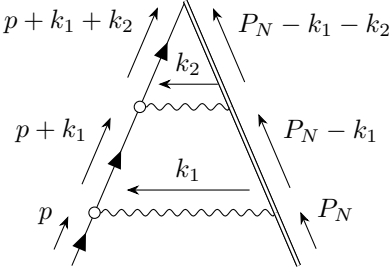
$$= -4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} [e^{-i\mathbf{k}_2 \cdot \mathbf{x}} - 1] \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{(\mathbf{k}_1 + \mathbf{k}_2)^2 / 8m^2}{|\mathbf{k}_2|^2 - 2mE}$$


$$= -4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} [e^{-i\mathbf{k}_2 \cdot \mathbf{x}} - 1] \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{(\mathbf{p} + \mathbf{k}_1)^2 / 8m^2}{|\mathbf{k}_1|^2 - 2mE} \frac{1}{|\mathbf{k}_2|^2 - 2mE}$$

Appendices

A Local Matrix Elements

For any diagram with the structure of

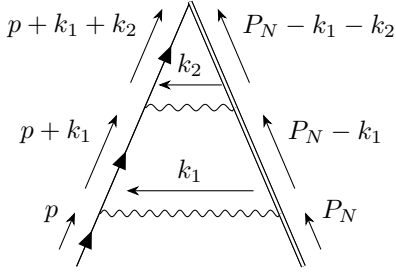


where the empty dot stands for any type of vertex involved, it can be written down as

$$= -4m^2 \mu^{2\epsilon} Z^2 e^4 \left[\int [dk_1][dk_2] \frac{1}{|\mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_2|^2} \frac{1}{-k_1^0 - k_2^0 + i\epsilon} \frac{1}{-k_1^0 + i\epsilon} \frac{1}{E + k_1^0 - \frac{(\mathbf{p} + \mathbf{k}_1)^2}{2m} + i\epsilon} \frac{1}{E + k_1^0 + k_2^0 - \frac{(\mathbf{p} + \mathbf{k}_1 + \mathbf{k}_2)^2}{2m} + i\epsilon} \right]$$

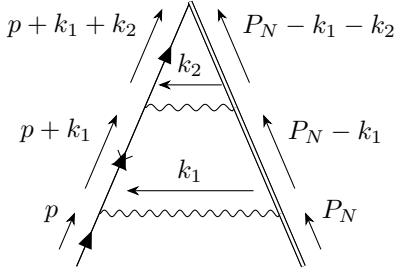
$$= -4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{1}{|\mathbf{k}_2|^2 - 2mE}$$

All diagrams at NNLO are



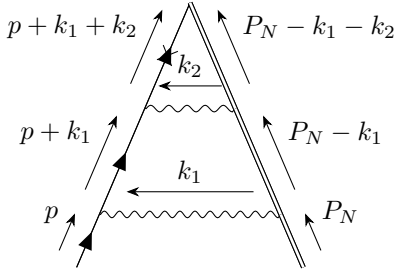
$$= -4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{1}{|\mathbf{k}_2|^2 - 2mE}$$

$$= 0 + \text{finite terms}$$



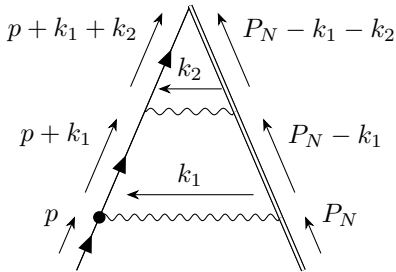
$$= -4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{(\mathbf{k}_1 + \mathbf{k}_2)^2 / 8m^2}{|\mathbf{k}_2|^2 - 2mE}$$

$$= Z^2 \alpha^2 \left(\frac{1}{2(3-d)} + \log \mu \right) + \text{finite terms}$$



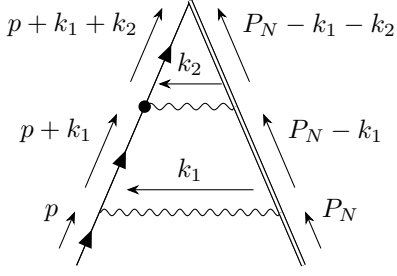
$$= -4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{(\mathbf{k}_1 + \mathbf{k}_2)^2 / 8m^2}{|\mathbf{k}_2|^2 - 2mE}$$

$$= 0 + \text{finite terms}$$



$$= -4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{(\mathbf{k}_1 + \mathbf{k}_2)^2 / 8m^2}{|\mathbf{k}_2|^2 - 2mE}$$

$$= Z^2 \alpha^2 \left(\frac{1}{4(d-3)} - \frac{\log \mu}{2} \right) + \text{finite terms}$$



$$\begin{aligned}
&= -4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{(\mathbf{k}_1 + \mathbf{k}_2)^2 / 8m^2}{|\mathbf{k}_2|^2 - 2mE} \\
&= Z^2 \alpha^2 \left(\frac{1}{2(d-3)} - \log \mu \right) + \text{finite terms}
\end{aligned}$$

References

- [Darwin(1928)] C. G. Darwin, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* **118**, 654 (1928).
- [Gordon(1928)] W. Gordon, *Zeitschrift für Physik* **48**, 11 (1928).
- [Bethe *et al.*(2008)Bethe, Salpeter, and Physics] H. A. Bethe, E. E. Salpeter, and Physics, *Quantum Mechanics of One- and Two-Electron Atoms (Dover Books on Physics)* (Dover Publications, 2008).