

# Divergence of Dirac Hydrogen Wavefunction Near Origin

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## Abstract

### INTRODUCTION

#### I. HYDROGEN WAVEFUNCTION DIVERGENCE NEAR ORIGIN IN DIRAC EQUATION AND SCHRÖDINGER EQUATION

##### A. 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 wavefunction[1] is[2-4]

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

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

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  $\psi_u$ , 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  $\Psi'$  is dimensionless and expand it in  $\alpha$ , 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  $\mu$ .

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## B. 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

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

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

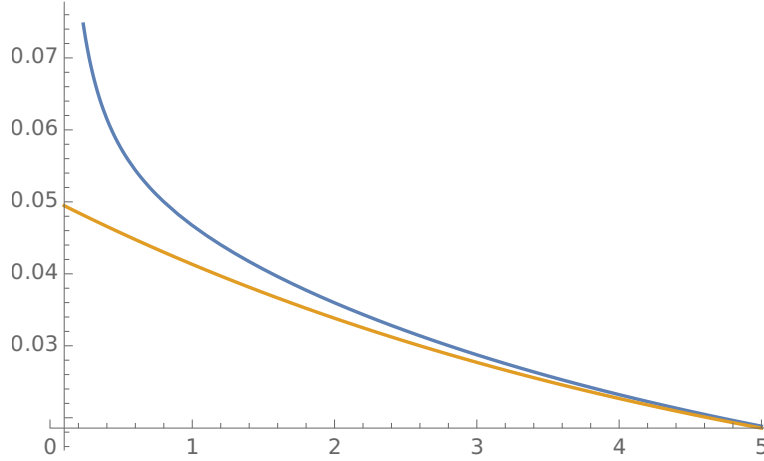


FIG. 1. Comparison between refactored Dirac wavefunction and Schrödinger wavefunction near origin.

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

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

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

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  $\kappa$  cutoff  $\Lambda$ , is

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

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

## II. NON-RELATIVISTIC QED (NRQED) MATCHING

### A. Feynman Rules

#### 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. 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

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.

## B. LO Matching

### 1. QED

In tree level[5]

## 2. NRQED

$$i\mathcal{M}_{NRQED}^{(0)} = \begin{array}{c} P_N \text{---} P_N \\ | \\ q \text{---} \\ | \\ p_1 \text{---} p_2 \end{array} = -e^2 \bar{u}_N(P_N) v^0 u_N(P_N) \frac{i}{\mathbf{q}^2} \psi^\dagger(p_2) \psi(p_1)$$

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 BBL[6].

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

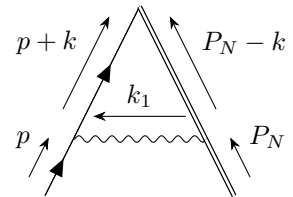
$$\left[ 1 - \frac{(\mathbf{p}_1 + \mathbf{p}_2)^2 - 2i(\mathbf{p}_1 \times \mathbf{p}_2) \cdot \boldsymbol{\sigma}}{8m^2} \right]$$

we can add additional vertexes

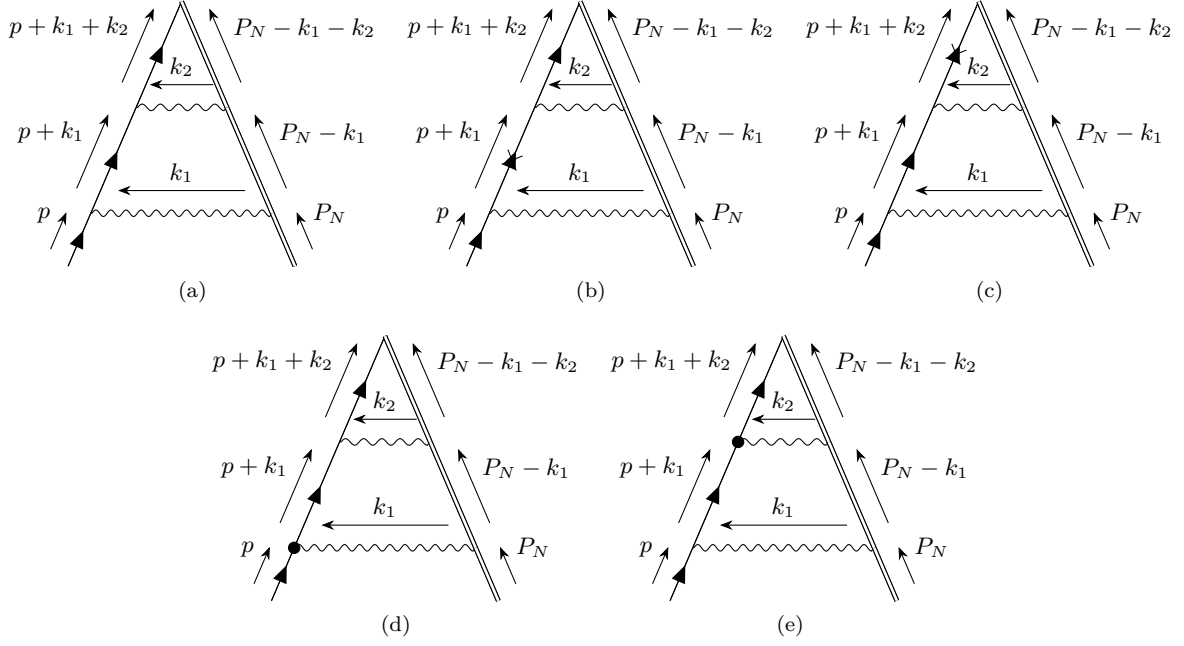
$$\begin{array}{c} p_2 \\ \nearrow \\ p_1 \text{---} \bullet \text{---} \\ \searrow \\ A^0 \end{array} = ie \frac{(\mathbf{p}_1 + \mathbf{p}_2)^2}{8m^2} \quad \text{and} \quad \begin{array}{c} p_2 \\ \nearrow \\ p_1 \text{---} \blacksquare \text{---} \\ \searrow \\ A^0 \end{array} = e \frac{(\mathbf{p}_1 \times \mathbf{p}_2) \cdot \boldsymbol{\sigma}}{4m^2} \quad (22)$$

## III. LOCAL OPERATOR AND MATRIX ELEMENT OF NRQED

### A. 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).



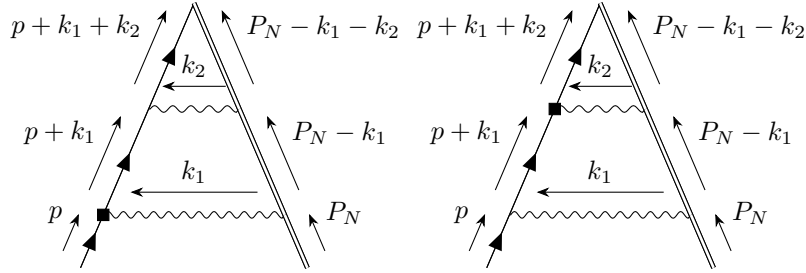
## B. NNLO

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

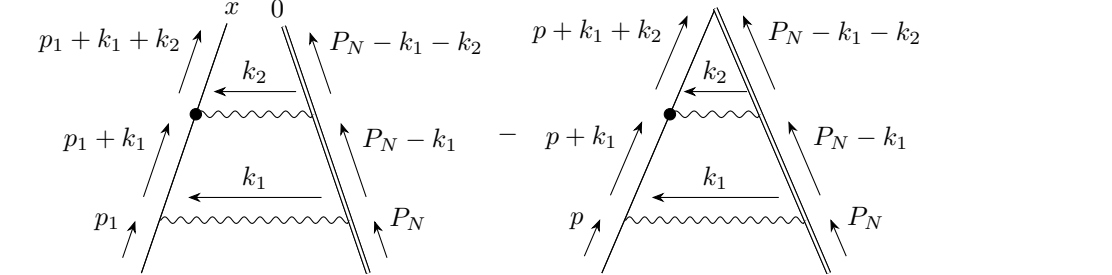


The first one gives  $\mathbf{p} \cdot (\boldsymbol{\sigma} \times \mathbf{p})$  and the second one ends up with  $\mathbf{k}_1 \cdot (\boldsymbol{\sigma} \times \mathbf{k}_1)$  after integrated the first loop so they're zero.

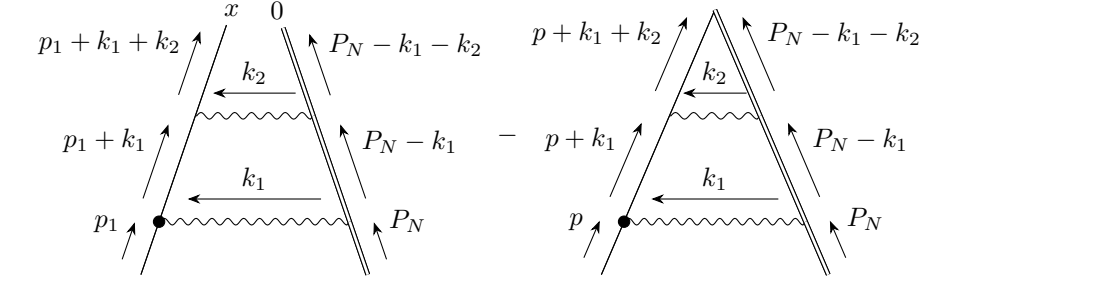
## IV. OPE

The relativistic correction part is the same as scalar ones.

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



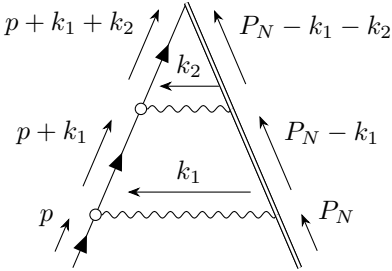
$$= -4m^2\mu^{2\epsilon}Z^2e^4 \int \frac{d^d\mathbf{k}_1}{(2\pi)^d} \frac{d^d\mathbf{k}_2}{(2\pi)^d} [e^{-i\mathbf{k}_2\cdot\mathbf{x}} - 1] \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{(\mathbf{k}_1 + \mathbf{k}_2)^2/8m^2}{|\mathbf{k}_2|^2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



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

## Appendix A: Local Matrix Elements

For any diagram with the structure of



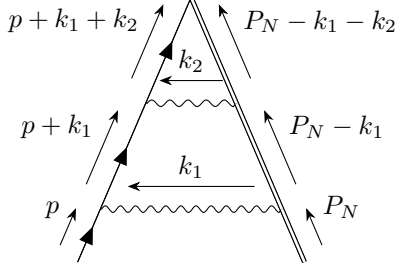
where the empty dot stands for any type of vertex involved, it can be written down as

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

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

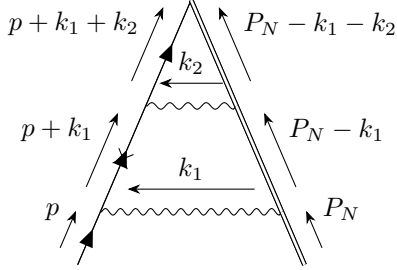


All diagrams at NNLO are



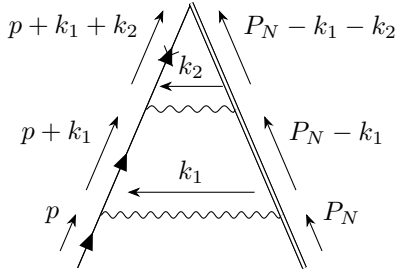
$$= -4m^2\mu^{2\epsilon}Z^2e^4 \int \frac{d^d\mathbf{k}_1}{(2\pi)^d} \frac{d^d\mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{1}{|\mathbf{k}_2|^2 - 2mE}$$

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



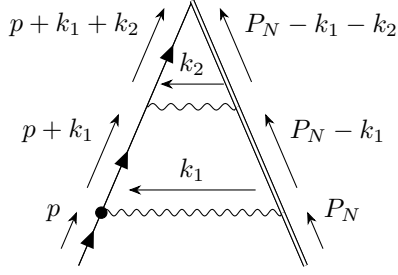
$$= -4m^2\mu^{2\epsilon}Z^2e^4 \int \frac{d^d\mathbf{k}_1}{(2\pi)^d} \frac{d^d\mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{(\mathbf{k}_1 + \mathbf{k}_2)^2/8m^2}{|\mathbf{k}_2|^2 - 2mE}$$

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

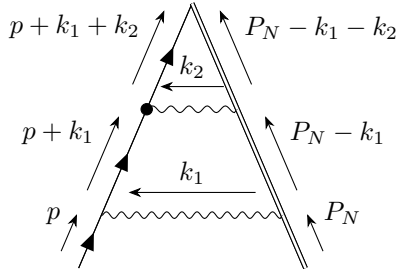


$$= -4m^2\mu^{2\epsilon}Z^2e^4 \int \frac{d^d\mathbf{k}_1}{(2\pi)^d} \frac{d^d\mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{(\mathbf{k}_1 + \mathbf{k}_2)^2/8m^2}{|\mathbf{k}_2|^2 - 2mE}$$

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



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



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

- 
- [1] This wavefunction checks out with Bethe's, except for an extra  $i$ .
- [2] C. G. Darwin, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* **118**, 654 (1928).
- [3] W. Gordon, *Zeitschrift für Physik* **48**, 11 (1928).
- [4] H. A. Bethe, E. E. Salpeter, and Physics, *Quantum Mechanics of One- and Two-Electron Atoms (Dover Books on Physics)* (Dover Publications, 2008).
- [5] Note that there's no Gamma matrix in the heavy particle side, they can only appear in the QED side.
- [6] Which contains both Darwin and spin-orbital terms.