Scalar QED

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Hydrogen Wavefunction Divergence Near Origin in Klein-Gordon Equation 1 and Schrödinger Equation

The Klein-Gordon part 1.1

The Klein-Gordon Hydrogen Equation is

$$\left(\left(i\partial_0 + \frac{Z\alpha}{r}\right)^2 + \nabla^2 - m^2\right)\Psi = 0\tag{1}$$

For the bound state, the eigen value and the wave function are

$$E = m \frac{1}{\sqrt{1 + \frac{\alpha^2 Z^2}{(\frac{1}{2} + \sqrt{\frac{1}{4} - Z^2 \alpha^2})^2}}}$$

$$\Psi = \frac{c}{\sqrt{4\pi}} e^{-kr} r^{\lambda}$$
(3)

$$\Psi = \frac{c}{\sqrt{4\pi}} e^{-kr} r^{\lambda} \tag{3}$$

where

$$\lambda = -\frac{1}{2} + \sqrt{\frac{1}{4} - Z^2 \alpha^2} \qquad c = \sqrt{\frac{(2k)^{2(1+\sqrt{\frac{1}{4} - Z^2 \alpha^2})}}{\Gamma(2 + 2\sqrt{\frac{1}{4} - Z^2 \alpha^2}))}} \qquad k = \frac{m}{\sqrt{1 + \frac{(\frac{1}{2} + \sqrt{\frac{1}{4} - Z^2 \alpha^2})^2}{\alpha^2 Z^2}}}$$
(4)

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

$$\Psi' = \frac{\Psi}{2(mZ\alpha)^{\frac{3}{2}}} \tag{5}$$

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

$$-(Z\alpha)^2\log(mr)\tag{6}$$

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

1.2 The Schrödinger part

The Hamiltonian is

$$H = H_0 + H_{int} \tag{7}$$

$$H_0 = -\frac{\nabla^2}{2m} - \frac{Z\alpha}{r}, \quad H_{int} = \frac{\nabla^4}{8m^3} + \frac{1}{32m^4} [-\nabla^2, [-\nabla^2, -\frac{Z\alpha}{r}]]$$
 (8)

The first term of H_{int} is the relativistic kinematic v^2 correction, the second one is the Darwin term. The H_0 gives the radial wave functions as follows

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

$$R_{k0} = \sqrt{\frac{2}{\pi}} (mZ\alpha)^{\frac{3}{2}} k e^{\frac{\pi}{2k}} |\Gamma(1 - \frac{i}{k})| e^{-imz\alpha kr} F(1 + \frac{i}{k}, 2, 2imZ\alpha kr), \quad E_k = \frac{mZ^2\alpha^2 k^2}{2}$$
(10)

Within perturbation theory, $E_1^{(1)} = \langle \phi | H_{int} | \phi \rangle$, in quantum mechanics, the NLO energy correction is

$$E_1^{(1)} = E_1 Z^2 \alpha^2 \tag{11}$$

The NLO corretion of the bound state wave function is

$$\sum_{n \neq 1} a_{n1}\phi_{n00} + \int dk a_{k1}\phi_{k00} \tag{12}$$

with

$$a_{n1} = \frac{\langle \phi_{n00} | H_{int} | \phi_{100} \rangle}{E_1 - E_n} \tag{13}$$

the discrete part of (12) is not divergent at r=0. We now focus on the integration part and seperate the relativistic kinematic term and the Darwin term. Since we are only interested in the divergent part, here we give a hard cutoff $\frac{\Lambda}{m}$ as the up-limit of the integration and a also a down-limit λ , with $\lambda >> 1$ (note that the following wave function have been multiplied by $2(mZ\alpha)^{\frac{3}{2}}$)

$$\Phi^{(1)}(0)_{kin} = \int_{\lambda}^{\frac{\Lambda}{m}} dk \frac{2Z^2 \alpha^2 k^{\frac{3}{2}}}{2\pi(\sqrt{1 - \exp(-\frac{2\pi}{k})})} \left(1 - \frac{2}{1 + k^2} \exp\left(-\frac{2\arctan(k)}{k}\right)\right) e^{\frac{\pi}{2k}} |\Gamma(1 - \frac{i}{k})|$$
(14)

with the integral region we defined (k >> 1), it would be OK to expand the integrand in $\frac{1}{k}$ (I havn't prove it yet), then the UV divergent term is

$$\Phi^{(1)}(0)_{kin} = \int_{\lambda}^{\frac{\Lambda}{m}} dk (Z\alpha)^2 (\frac{1}{\pi} + \frac{1}{k})$$
 (15)

$$\sim (\alpha Z)^2 \left(\frac{\Lambda}{\pi m} + \log\left(\frac{\Lambda}{m}\right)\right) \tag{16}$$

The UV divergent part of Darwin term is

$$\Phi^{(1)}(0)_D = -\frac{(Z\alpha)^4}{8\pi} \int_{\lambda}^{\frac{\Lambda}{m}} dk k^2 e^{\frac{\pi}{k}} |\Gamma(1 - \frac{i}{k})|^2$$
(17)

with the same trick as (15), the UV divergen part is

$$\Phi^{(1)}(0)_D = -(\alpha Z)^4 \int_{1}^{\frac{\Lambda}{m}} dk \frac{k^2}{8\pi} + \frac{k}{8} + \frac{1}{24}\pi$$
 (18)

$$\sim -\frac{(Z\alpha)^4}{8\pi} (\frac{\Lambda^3}{3m^3} + \frac{\pi\Lambda^2}{2m^2} + \frac{\pi^2\Lambda}{3m})$$
 (19)

Now collect all the results we get as follow.

The K-G wave function's origin UV divergence is

$$K - G \quad UV : -(Z\alpha)^2 \log(mr) \tag{20}$$

The purterbative Schrödinger wave function's origin UV divergence, with a k cutoff $\frac{\Lambda}{m}$, is

$$Kin\ UV: (\alpha Z)^2(\frac{\Lambda}{\pi m} + \log\left(\frac{\Lambda}{m}\right))$$
 (21)

Darwin
$$UV : -\frac{(Z\alpha)^4}{8\pi} (\frac{\Lambda^3}{3m^3} + \frac{\pi\Lambda^2}{2m^2} + \frac{\pi^2\Lambda}{3m})$$
 (22)

All the m, under Λ or in a log, can be interpreted as a subtraction point μ .

2 Non-relativistic Scalar QED (NRSQED) Matching

2.1 Feynman Rules

2.1.1 Scalar QED (SQED)

Lagrangian

$$\mathcal{L}_{SQED} = |D_{\mu}\phi|^2 - m^2 |\phi|^2 + \Phi_v^* i v \cdot D\Phi_v$$
(23)

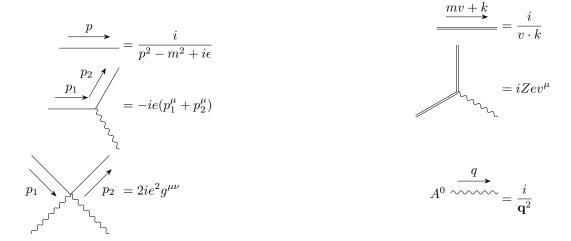
with

$$D_{\mu}\phi = \partial_{\mu}\phi + ieA_{\mu}\phi$$

and

$$D_{\mu}\Phi_{\nu} = \partial_{\mu}\Phi - iZeA_{\mu}\Phi_{\nu}$$

But note that no A can appear in actual calculation because here only static scalar potential exists. And the Feynman rules



2.1.2 **NRSQED**

Using the transformation $\phi \to \frac{e^{-imt}}{\sqrt{2m}}\varphi$, we can have the Lagrangian

$$\mathcal{L}_{NRSQED} = \varphi^* \left(iD_0 + \frac{\mathbf{D}^2}{2m} \right) \varphi + \delta \mathcal{L} + \Phi_v^* iv \cdot D\Phi_v$$
 (24)

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} .

Since we need to match it to $\mathcal{O}(v^2)$ order

$$\delta \mathcal{L} = \frac{(D_0 \varphi)^* (D_0 \varphi)}{2m} = \frac{\dot{\varphi}^* \dot{\varphi}}{2m} + \frac{e^2 \varphi^* \varphi A_0^2}{2m} - \frac{ie}{2m} A_0 (\varphi^* \dot{\varphi} - \dot{\varphi}^* \varphi) \tag{25}$$

and it changes the Feynman rules to¹

$$\begin{array}{c} p_2 \\ p_1 \\ \hline \\ A^0 \end{array} = -ie(1 + \frac{E_1 + E_2}{2m}) \qquad p_1 \\ \hline \\ A^0 \qquad A^0 \qquad A^0 \end{array} = \frac{ie^2}{2m}$$

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Since we rescaled ϕ by $\frac{1}{\sqrt{2m}}$ to get φ , the in/out states are also changed. We must multiply them by $\sqrt{2p^0}$ to compensate that change.

Another way to achieve it is to use the transform rules of heavy scalar effective theory (HSET).

In this note, p^0 is the zero component of relativistic four momentum, and $E = p^0 - m$.

2.1.3 NRSQED-1

Let's focus on the lagrangian of only a single Scalar field

$$\mathcal{L}_{SQED} = |D_{\mu}\phi|^2 - m^2|\phi|^2 \tag{26}$$

Substitute ϕ for $\phi = \frac{1}{\sqrt{2m}} e^{-imv \cdot x} (\varphi_v + \bar{\varphi}_v)$ with (Schwartz, Sec 35.2)

$$\varphi_v = \frac{1}{\sqrt{2m}} e^{imv \cdot x} (iv \cdot D + m)\phi \tag{27}$$

$$\bar{\varphi}_v = \frac{1}{\sqrt{2m}} e^{imv \cdot x} (-iv \cdot D + m)\phi \tag{28}$$

then

$$\mathcal{L}_{SQED} = \frac{1}{2m} (D_{\mu}(\varphi_v + \bar{\varphi}_v))^* D^{\mu}(\varphi_v + \bar{\varphi}_v) + (\varphi_v + \bar{\varphi}_v)^* iv \cdot D(\varphi + \bar{\varphi}_v)$$
(29)

Within our calculation, we set $\vec{A} = 0, v = (1, \vec{0})$. Then from (25), (26) and the motion equation derived from (27), we get two equation

$$\bar{\varphi}_v = \frac{-iD_0}{2m}(\varphi_v + \bar{\varphi}_v) \tag{30}$$

$$\frac{-iD_0}{2m}\varphi_v = \frac{\nabla^2}{4m^2}(\varphi_v + \bar{\varphi}_v) \tag{31}$$

And (27) could be transformed as

$$\mathcal{L}_{SQED} = (\varphi_v + \bar{\varphi}_v)^* (iD_0 + \frac{\nabla^2}{2m} - \frac{D_0^2}{2m})(\varphi + \bar{\varphi}_v)$$
(32)

Substituting (28), (29) iteratively, then we get the \mathcal{L} expanding for v as

$$\mathcal{L}_{SQED} = \varphi_v^* (iD_0 + \frac{\nabla^2}{2m} + \frac{\nabla^4}{8m^3} + \frac{\nabla^6}{16m^5} + \frac{e}{32m^4} ([\nabla^2, [A_0, \nabla^2]] + [A_0, \nabla^4]) + \mathcal{O}(v^7))\varphi_v$$
(33)

2.2 LO Matching

2.2.1 SQED

$$i\mathcal{M}_{SQED}^{(0)} = \begin{array}{c} P_N = P_N \\ \downarrow \\ p_1 = P_2 \end{array} = -e^2 v^0 \frac{i(p_1^0 + p_2^0)}{\mathbf{q}^2} = -e^2 v^0 \frac{i}{\mathbf{q}^2} (2m + 2E_1)$$

2.2.2 NRSQED

$$i\mathcal{M}_{NRSQED}^{(0)} = \begin{array}{c} P_N \\ \hline \\ p_1 \end{array} = -2\sqrt{p_1^0 p_2^0} e^2 v^0 \frac{i(1+\delta)}{\mathbf{q}^2} = -e^2 v^0 \times 2p_1^0 \frac{i(1+\delta)}{\mathbf{q}^2} \\ \hline \\ p_2 \end{array}$$

which gives

$$\delta = \frac{p_1^0 + p_2^0}{2\sqrt{p_1^0 p_2^0}i} - 1 \approx \frac{\mathbf{p}_1^4 - 2\mathbf{p}_1^2 \mathbf{p}_2^2 + \mathbf{p}_2^4}{32m^4}$$

The new electron-photon vertex is

$$= i + i \frac{\mathbf{p}_1^4 - 2\mathbf{p}_1^2\mathbf{p}_2^2 + \mathbf{p}_2^4}{32m^4}$$

$$A^0$$

We can write the correction interacting term corresponding to δ as

$$A_0 \varphi \nabla^4 \varphi^* - 2A_0 \nabla^2 \varphi^* \nabla^2 \varphi + \varphi^* A_0 \nabla^4 \varphi = \varphi^* \nabla^4 (A_0 \varphi) - 2\varphi^* \nabla^2 (A_0 \nabla^2 \varphi) + \varphi^* A_0 \nabla^4 \varphi$$
$$= \varphi^* (\nabla^2 [\nabla^2, A_0] - [\nabla^2, A_0] \nabla^2) \varphi$$
$$= \varphi^* [\nabla^2, [\nabla^2, A_0]] \varphi$$

which is exactly the Darwin term in Holstein's Advanced Topics in QM with coefficient $1/32m^4$.

3 Local Operator and Matrix Element of NRSQED

To reproduce the singular behavior of "Klein-Gordon Hydrogen" wavefunction near origin, we can try OPE. But the dependence of x in OPE can be taken as a regularization scheme and thus the result should be the same as local one without renormalization. And the logarithmic terms of x in OPE can be reproduced by the logarithmic divergence of local operators. Since in the study of Klein-Gordon equation we know that the wavefunction only contains logarithmic divergence at the origin so that's the only type of divergence we're looking for.

3.1 LO

3.2 NLO

$$\langle 0|\psi_e(0)N(0)(-ie\mu^{-\epsilon})\int \mathrm{d}^4y\bar{\psi}_e\psi_eA^0(-ie\mu^{-\epsilon})\int \mathrm{d}^4z\bar{N}NA^0|eN\rangle = p + k P_N - k$$

$$p + k P_N - k$$

$$p + k P_N - k$$

$$p + k P_N - k$$

which doesn't have logarithm divergence².

²After dimensional regularization, the Gamma function in the numerator is something like $\Gamma(n-d/2)$ and Gamma function doesn't have pole at half integer. We can rigorously prove this kind of diagrams do not have logarithmic divergence at one loop.

3.3 **NNLO**

$$p + k_{1} + k_{2}$$

$$p + k_{1}$$

$$p + k_{1$$

do the shift as above

$$= \mu^{2\epsilon} Z^2 e^4 \left[\int \frac{\mathrm{d}^3 \mathbf{k_1}}{(2\pi)^3} \frac{\mathrm{d}^3 \mathbf{k_2}}{(2\pi)^3} \frac{1}{\left|\mathbf{k_1} - \mathbf{p}\right|^2} \frac{1}{\left|\mathbf{k_2} - \mathbf{k_1}\right|^2} \frac{1}{E - \frac{\left|\mathbf{k_1}\right|^2}{2m} + 2i\epsilon} \frac{1}{E - \frac{\left|\mathbf{k_2}\right|^2}{2m} + 2i\epsilon} \right] = 0$$

$$p + k_1 + k_2 +$$

$$p + k_{1} + k_{2} + k_{2} + k_{1} + k_{2} +$$

=0 + finite terms

Appendices

A Useful formulas in Feynman integrals

Feynman parametrization used here is

$$\frac{1}{\prod A_i^{d_i}} = \int \prod dx_i \delta(\sum x_i - 1) \frac{\prod x_i^{d_i - 1}}{\left[\sum x_i A_i\right]^{\sum d_i}} \frac{\Gamma(\sum d_i)}{\prod \Gamma(d_i)}$$
(34)

Integral with the structure of the form

$$\int [dk_1][dk_2] \frac{1}{|\mathbf{k_1}|^2} \frac{1}{|\mathbf{k_2}|^2} \frac{1}{-k_1^0 - k_2^0 + i\epsilon} \frac{1}{-k_1^0 + i\epsilon} \frac{1}{[p^0 + k_1^0 - M - \frac{(\mathbf{p} + \mathbf{k_1})^2}{2M} + i\epsilon]^m} \frac{1}{[p^0 + k_1^0 + k_2^0 - M - \frac{(\mathbf{p} + \mathbf{k_1} + \mathbf{k_2})^2}{2M} + i\epsilon]^n}$$

will always produce

$$\int \frac{\mathrm{d}^3\mathbf{k_1}}{(2\pi)^3} \frac{\mathrm{d}^3\mathbf{k_2}}{(2\pi)^3} \frac{1}{|\mathbf{k_1}|^2} \frac{1}{|\mathbf{k_2}|^2} \frac{1}{[p^0 - M - \frac{(\mathbf{p} + \mathbf{k_1})^2}{2M}]^m} \frac{1}{[p^0 - M - \frac{(\mathbf{p} + \mathbf{k_1} + \mathbf{k_2})^2}{2M} + i\epsilon]^n}$$

with k_1^0 and k_2^0 goes to zero.

For arbitary one loop diagram of the following form, we have

$$\int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{k^{2\beta}}{(k^2 + \Delta)^n} = \frac{1}{(4\pi)^{n-\beta}} \frac{\Gamma(\beta + d/2)}{\Gamma(d/2)} \frac{\Gamma(n - \beta - d/2)}{\Gamma(n)} \left(\frac{4\pi}{\Delta}\right)^{n-\beta - d/2}$$
(35a)

$$= \frac{1}{(4\pi)^{d/2}} \frac{\Gamma(\beta + d/2)}{\Gamma(d/2)} \frac{\Gamma(n - \beta - d/2)}{\Gamma(n)} \left(\frac{1}{\Delta}\right)^{n - \beta - d/2}$$
(35b)

where $\frac{1}{(4\pi)^{d/2}}$ often appears as $2^{-d}\pi^{-d/2}$.

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