

Divergence of Klein-Gordon Hydrogen Wavefunction Near Origin

Yingsheng Huang and Rui Yu

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Introduction

1 Divergence in Klein-Gordon Equation and Schrödinger Equation

1.1 Klein-Gordon Equation Coulomb Potential Solution

In this section we revisit the divergence of wavefunction near origin in the framework of quantum mechanics.

The Klein-Gordon Hydrogen Equation is

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

For the bound state, the eigen value and the wave function are [1]

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

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

where

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

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

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

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

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

$$\Psi(\mathbf{r}) \sim -(Z\alpha)^2 \log(2mZ\alpha r) / \sqrt{4\pi} \quad (7)$$

the m in log could be interpreted as a subtraction point μ . This divergence is discussed by many papers [2,3].

1.2 The Schrödinger part

By taking the non-relativistic limit of Klein-Gordon Hydrogen Hamiltonian, the effective Schrödinger Hamiltonian is [4]

$$H = H_0 + H_{int}, \quad H_{int} = H_{kin} + H_{Darwin} + \mathcal{O}(v^6) \quad (8)$$

$$H_0 = -\frac{\nabla^2}{2m} - \frac{Z\alpha}{r}, \quad H_{kin} = \frac{\nabla^4}{8m^3}, \quad H_{Darwin} = \frac{1}{32m^4}[-\nabla^2, [-\nabla^2, -\frac{Z\alpha}{r}]] \quad (9)$$

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

$$R_{n0} = \frac{2(mZ\alpha)^{\frac{3}{2}}}{n^{\frac{3}{2}}} e^{-\frac{mZ\alpha}{n}r} F(1-n, 2, \frac{2mZ\alpha r}{n}), \quad E_n = -\frac{Z^2\alpha^2 m}{2n^2} \quad (10)$$

$$R_{\kappa 0} = \sqrt{\frac{2}{\pi}} (mZ\alpha)^{\frac{3}{2}} \kappa e^{\frac{\pi}{2\kappa}} |\Gamma(1 - \frac{i}{\kappa})| e^{-imZ\alpha\kappa r} F(1 + \frac{i}{\kappa}, 2, 2imZ\alpha\kappa r), \quad E_\kappa = \frac{mZ^2\alpha^2\kappa^2}{2} \quad (11)$$

where the relation between dimensionless κ and the actual momentum \mathbf{k} is $\kappa = \frac{|\mathbf{k}|}{mZ\alpha}$, and the normalization of continuum spectrum is followed by

$$\int r^2 dr R_{\kappa'l} R_{\kappa l} = \delta(k' - k).$$

The NLO correction of the bound state wave function is

$$\sum_{n \neq 1} a_{n1} \phi_{n00} + \int d\kappa a_{1\kappa} \phi_{\kappa 00} \quad (12)$$

with

$$a_{n1} = \frac{\langle \phi_{n00} | H_{kin} | \phi_{100} \rangle}{E_1 - E_n} = \frac{2\alpha^2 \sqrt{n} \left(\left(2 \left(\frac{n-1}{n+1} \right)^n - 1 \right) n^2 + 1 \right) Z^2}{(n^2 - 1)^2}$$

and

$$a_{\kappa 1} = \frac{\langle \phi_{\kappa 00} | H_{kin} | \phi_{100} \rangle}{E_1 - E_\kappa} = \frac{2\alpha^2 \sqrt{\kappa} Z^2 \left(\frac{(\kappa^2 - 1)e^{-\frac{2 \tan^{-1}(\kappa)}{\kappa}}}{\kappa^2 + 1} - e^{-\frac{2 \tan^{-1}(\kappa)}{\kappa}} + 1 \right)}{\sqrt{1 - e^{-\frac{2\pi}{\kappa}}} (\kappa^2 + 1)}$$

the discrete part of (12) is not divergent at $r = 0$. We now focus on the integration part and separate 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 (note that the following wave function have been multiplied by $2(mZ\alpha)^{\frac{3}{2}}$)

$$\Phi^{(1)}(0)_{kin} = \int^{\frac{\Lambda}{m}} d\kappa \frac{2Z^2\alpha^2\kappa^{\frac{3}{2}}}{2\pi(\sqrt{1 - \exp(-\frac{2\pi}{\kappa})})} \left(1 - \frac{2}{1 + \kappa^2} \exp\left(-\frac{2 \arctan(\kappa)}{\kappa}\right) \right) e^{\frac{\pi}{2\kappa}} |\Gamma(1 - \frac{i}{\kappa})| \quad (13)$$

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

$$R^{(1)}(0)_{kin} = \int^{\frac{\Lambda}{m}} d\kappa (Z\alpha)^2 \left(\frac{1}{\pi} + \frac{1}{\kappa} \right) \quad (14)$$

$$\sim (\alpha Z)^2 \left(\frac{\Lambda}{\pi m} + \log \left(\frac{\Lambda}{m} \right) \right) \quad (15)$$

For Darwin term

$$a_{n1} = \frac{\langle \phi_{n00} | H_{Darwin} | \phi_{100} \rangle}{E_1 - E_n} = \frac{\alpha^4 Z^4}{4n^{3/2}}$$

$$a_{\kappa 1} = \frac{\langle \phi_{\kappa 00} | H_{Darwin} | \phi_{100} \rangle}{E_1 - E_\kappa} = \frac{1}{4} \alpha^4 e^{\frac{\pi}{2\kappa}} \kappa Z^4 \left| \Gamma \left(1 - \frac{i}{\kappa} \right) \right|$$

The UV divergent part of Darwin term is

$$R^{(1)}(0)_D = -\frac{(Z\alpha)^4}{8\pi} \int^{\frac{\Lambda}{m}} d\kappa \kappa^2 e^{\frac{\pi}{2\kappa}} \left| \Gamma \left(1 - \frac{i}{\kappa} \right) \right|^2 \quad (16)$$

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

$$R^{(1)}(0)_D = -(\alpha Z)^4 \int_{\lambda}^{\frac{\Lambda}{m}} d\kappa \frac{\kappa^2}{8\pi} + \frac{\kappa}{8} + \frac{1}{24}\pi \quad (17)$$

$$\sim -\frac{(Z\alpha)^4}{8\pi} \left(\frac{\Lambda^3}{3m^3} + \frac{\pi\Lambda^2}{2m^2} + \frac{\pi^2\Lambda}{3m} \right) \quad (18)$$

Now collect all the results we get as follows.

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

$$K - G \text{ UV} : -(Z\alpha)^2 \log(mr) \quad (19)$$

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

$$Kin \text{ UV} : (\alpha Z)^2 \left(\frac{\Lambda}{\pi m} + \log \left(\frac{\Lambda}{m} \right) \right) \quad (20)$$

$$Darwin \text{ UV} : -\frac{(Z\alpha)^4}{8\pi} \left(\frac{\Lambda^3}{3m^3} + \frac{\pi\Lambda^2}{2m^2} + \frac{\pi^2\Lambda}{3m} \right) \quad (21)$$

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

2 Scalar Non-relativistic QED (Scalar NRQED) Matching

In the following sections we work on the quantum field theory side. We'll use scalar NRQED to describe scalar electron and heavy scalar effective theory (HSET) to describe nucleus. But first, we'll need the Feynman rules of them.

2.1 Feynman Rules

2.1.1 Scalar QED (SQED)

The Lagrangian of scalar QED (HSET included) is

$$\mathcal{L}_{SQED} = |D_\mu \phi|^2 - m^2 |\phi|^2 + \Phi_v^* i v \cdot D \Phi_v \quad (22)$$

with the covariant derivative defined as

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

and

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

But note that no dynamic electromagnetic field \mathbf{A} can appear in actual calculation because here only static scalar potential exists.

And the Feynman rules are

The Feynman rules for Scalar QED (SQED) are as follows:

- Propagator: $\frac{i}{p^2 - m^2 + i\epsilon}$
- Vertex (scalar-scalar-photon): $-ie(p_1^\mu + p_2^\mu)$
- Vertex (photon-photon): $2ie^2 g^{\mu\nu}$
- Vertex (scalar-photon): $\frac{i}{v \cdot k}$
- Photon propagator: $\frac{i}{\mathbf{q}^2}$

2.1.2 Scalar NRQED

Using the transformation $\phi \rightarrow \frac{e^{-imt}}{\sqrt{2m}} \varphi$, we can have the Lagrangian of scalar NRQED (HSET included)

$$\mathcal{L}_{SNRQED} = \varphi^* \left(iD_0 + \frac{\mathbf{D}^2}{2m} \right) \varphi + \delta\mathcal{L} + \Phi_v^* i v \cdot D \Phi_v \quad (23)$$

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 Feynman rules for Scalar NRQED are as follows:

- Propagator: $\frac{i}{E - \frac{\mathbf{p}^2}{2m} + i\epsilon}$
- Vertex (scalar-scalar-photon): $-ie$

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

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

$$\delta\mathcal{L} = \frac{(D_0\varphi)^*(D_0\varphi)}{2m} = \frac{\dot{\varphi}^*\dot{\varphi}}{2m} + \frac{e^2\varphi^*\varphi A_0^2}{2m} - \frac{ie}{2m}A_0(\varphi^*\dot{\varphi} - \dot{\varphi}^*\varphi) \quad (24)$$

and it changes the Feynman rules to¹

$$\begin{aligned} \text{Diagram 1: } & \text{Feynman rule for } A^0 \text{ vertex: } -ie\left(1 + \frac{E_1 + E_2}{2m}\right) \\ \text{Diagram 2: } & \text{Feynman rule for } A^0 \text{ vertex: } \frac{ie^2}{2m} \end{aligned}$$

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).

2.1.3 Scalar NRQED Lagrangian via HSET transformation

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

$$\mathcal{L}_{SQED} = |D_\mu\phi|^2 - m^2|\phi|^2 \quad (25)$$

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

$$\varphi_v = \frac{1}{\sqrt{2m}}e^{imv\cdot x}(iv\cdot D + m)\phi \quad (26)$$

$$\bar{\varphi}_v = \frac{1}{\sqrt{2m}}e^{imv\cdot x}(-iv\cdot D + m)\phi \quad (27)$$

then

$$\mathcal{L}_{SQED} = \frac{1}{2m}(D_\mu(\varphi_v + \bar{\varphi}_v))^*D^\mu(\varphi_v + \bar{\varphi}_v) + (\varphi_v + \bar{\varphi}_v)^*iv\cdot D(\varphi_v + \bar{\varphi}_v) \quad (28)$$

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

$$\bar{\varphi}_v = \frac{-iD_0}{2m}(\varphi_v + \bar{\varphi}_v) \quad (29)$$

$$\frac{-iD_0}{2m}\varphi_v = \frac{\nabla^2}{4m^2}(\varphi_v + \bar{\varphi}_v) \quad (30)$$

And (27) could be transformed as

$$\mathcal{L}_{SQED} = (\varphi_v + \bar{\varphi}_v)^*(iD_0 + \frac{\nabla^2}{2m} - \frac{D_0^2}{2m})(\varphi_v + \bar{\varphi}_v) \quad (31)$$

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

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

¹In this note, p^0 is the zero component of relativistic four momentum, and $E = p^0 - m$.

2.2 LO Matching

2.2.1 SQED

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

2.2.2 Scalar NRQED

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

which gives

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

The extra electron-photon vertex is

$$\begin{array}{c} p_2 \nearrow \\ p_1 \rightarrow \bullet \\ \searrow A^0 \end{array} = -i \frac{\mathbf{p}_1^4 - 2\mathbf{p}_1^2 \mathbf{p}_2^2 + \mathbf{p}_2^4}{32m^4}$$

We can write the correction interacting term corresponding to δ as

$$\begin{aligned} A_0 \varphi \nabla^4 \varphi^* - 2A_0 \nabla^2 \varphi^* \nabla^2 \varphi + \varphi^* A_0 \nabla^4 \varphi &= \varphi^* \nabla^4 (A_0 \varphi) - 2\varphi^* \nabla^2 (A_0 \nabla^2 \varphi) + \varphi^* A_0 \nabla^4 \varphi \\ &= \varphi^* (\nabla^2 [\nabla^2, A_0] - [\nabla^2, A_0] \nabla^2) \varphi \\ &= \varphi^* [\nabla^2, [\nabla^2, A_0]] \varphi \end{aligned}$$

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

Since there's no logarithmic divergence in one loop (which we'll mention it soon), we don't need to match the effective couplings to the next order. Even if we do so, in α^2 order, higher order corrections of interactions can only appear in one-loop or tree level. Next step, we'll calculate the logarithmic divergence of local matrix elements.

3 Local Operator and Matrix Element of Scalar NRQED

Assuming the full theory of the scalar electron is scalar QED, we can mimic the effect of nucleus, or rather to say, Coulomb potential, with heavy scalar effective theory, as mentioned before. For simplicity, and also the

goal of replicating divergence produced by Klein-Gordon equation, there's no need involving any other effect the nucleus might have. And as pointed out by Bodwin, Braaten and Lepage in 1995 [5], when discussing heavy quarkonium problem, non-relativistic Coulomb gauge wavefunction can be defined as NRQCD Bethe-Salpeter QQ wavefunction, evaluated at equal time. As an analogy, we can define NRQED wavefunction in the same fashion. Therefore, we can describe the radial wavefunction in terms of a matrix element

$$R(x) = \langle 0 | \psi(x) N(0) | atom \rangle. \quad (33)$$

We think that the divergence of wavefunction comes from the non-local attribute of operator $\psi(x)N(0)$ rather than the state $|atom\rangle$ itself, so it can be analyzed by operator product expansion (OPE) [6]. Therefore, we can transform the problem to another matrix element² (note that OPE is relations between operators, thus independent of where these operators are located at)

$$\langle 0 | \psi(x) N(0) \tilde{\psi}(p) \tilde{N}(k) | 0 \rangle = \int \frac{d^4 p}{(2\pi)^4} \frac{d^4 k}{(2\pi)^4} e^{-ip \cdot y} e^{-ik \cdot z} \langle 0 | \psi(x) N(0) \psi(y) N(z) | 0 \rangle. \quad (34)$$

To reproduce the singular behavior of “Klein-Gordon Hydrogen” wavefunction near origin, we could try OPE. But the dependence of x in this non-local matrix element can also be taken as a regularization scheme and thus the result should be the same as local one

$$\langle 0 | \psi(0) N(0) \tilde{\psi}(p) \tilde{N}(k) | 0 \rangle$$

without renormalization (except for the choice of different regulators). And the logarithmic terms of x in (33) can be reproduced by the logarithmic divergence of local operators. From what we learned in the discussion of Klein-Gordon equation in quantum mechanics, we know that the wavefunction only contains logarithmic divergence at the origin so that's the only type of divergence we're looking for. In this section, we'll isolate the logarithmic divergence using dimensional regularization, and reproduce what we obtained in quantum mechanics perturbation theory.

Intuitively, we can assume $\psi(x)$ is just the scalar field operator in scalar QED. But what we need is logarithmic divergence start at $Z^2 \alpha^2$ order, and using relativistic scalar field operator will result in logarithmic divergence at $Z \alpha$ order, which, since we already know the answer to the question, is not what we want. However, since QED, or in our case, scalar QED, has no bound on how small the distance it can probe, we might observe that in order to investigate low energy physics, we can't use theory with such sensitivity in short range.

The alternative is to use scalar NRQED on the scalar electron side. Through it's a non-relativistic theory thus not the first choice when studying a relativistic problem, the natural energy cutoff it provides will be very convenient in this problem.

First we define $\epsilon = 3 - d$ and on-shell momentum $P_N = m_N v_N$, also the momentum of scalar electron is $p = (E, \mathbf{p})$ and the momentum of nucleus is $P_N + k$.

3.1 NLO

It's obvious that the tree level has no divergence of any kind, so we'll start at one loop.

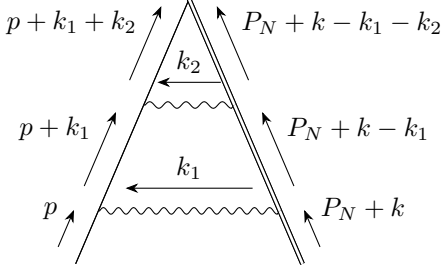
After dimensional regularization, the Gamma function in the numerator is something like $\Gamma(n - d/2)$ and Gamma function doesn't have pole at half integer. We can prove that any one-loop diagram involved does not have logarithmic divergence.

²Here the actual momentum of the nucleus is $P_N = m_N v_N$ but since m_N is decoupled in HSET, it can not appear anywhere in our calculations

3.2 NNLO

Since we're calculating Green function, the nucleus is off-shell by k . Although the effect is just a shift in electron energy (see Appendix B), it's convenient for us to redefine $E' = E + k^0$.

All the Feynman rules we need are derived above except for one: on the top of the diagram, the joint point stands for composite operator $\psi(0)N(0)$, whose Feynman rule is just 1; if it's separated a little, it stands for non-local fields in operator product expansion and can be treated as an exponential factor $e^{-i\mathbf{k}\cdot\mathbf{x}}$ where \mathbf{k} is the momentum of the cloest line in the electron side.



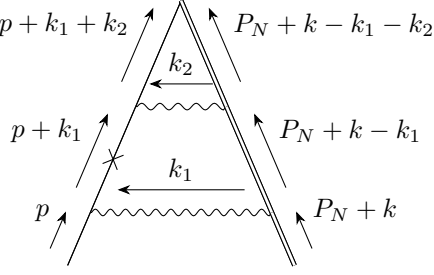
$$= -\mu^{2\epsilon} Z^2 e^4 \left[\int \frac{[dk_1]}{|\mathbf{k}_1|^2} \frac{[dk_2]}{|\mathbf{k}_2|^2} \frac{1}{k^0 - k_1^0 - k_2^0 + i\epsilon} \frac{1}{k^0 - k_1^0 + i\epsilon} \frac{1}{E + k_1^0 - \frac{(\mathbf{p}+\mathbf{k}_1)^2}{2m} + i\epsilon} \frac{1}{E + k_1^0 + k_2^0 - \frac{(\mathbf{p}+\mathbf{k}_1+\mathbf{k}_2)^2}{2m}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

integrate out the temporal component of loop momentum, then perform shifts $\mathbf{k}_1 \rightarrow \mathbf{k}_1 - \mathbf{p}$ and $\mathbf{k}_2 \rightarrow \mathbf{k}_2 - \mathbf{k}_1 - \mathbf{p}$ on them

$$\begin{aligned} &= \mu^{2\epsilon} Z^2 e^4 \left[\int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{E' - \frac{|\mathbf{k}_1|^2}{2m} + 2i\epsilon} \frac{1}{E' - \frac{|\mathbf{k}_2|^2}{2m} + 2i\epsilon} \right] \\ &= 4m^2 Z^2 \alpha^2 \mu^{2\epsilon} \int_0^1 dx_1 dx_2 \delta(x_1 + x_2 - 1) \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{[|\mathbf{k}_1|^2 - 2mE']^2} \frac{1}{\left(\mathbf{k}_1^2 - \frac{2mE}{x_1}\right)^{2-d/2}} \\ &\quad \left[2^{4-d} \pi^{2-\frac{d}{2}} (x_1 - x_1^2)^{\frac{d}{2}-2} \Gamma\left(2 - \frac{d}{2}\right) \right] \\ &= 4m^2 Z^2 \alpha^2 \mu^{2\epsilon} \int_0^1 dx_1 dx_2 dy_1 dy_2 dy_3 \delta(x_1 + x_2 - 1) \delta(y_1 + y_2 + y_3 - 1) \frac{2^{4-2d} \pi^{2-d} (x_1 - x_1^2)^{\frac{d}{2}-2} y_3^{1-\frac{d}{2}} \Gamma(4-d)}{\left(p^2 y_1 - p^2 y_1^2 - \frac{2mE y_3}{x_1} - 2mE y_2\right)^{4-d}} \\ &= \text{finite terms} \end{aligned}$$

Actually, after integrated the temporal part, we can determine from superficial divergence that unless the power of the numerator is higher than \mathbf{k}^2 , the diagram can not be divergent. We can do so by adding relativistic

corrections



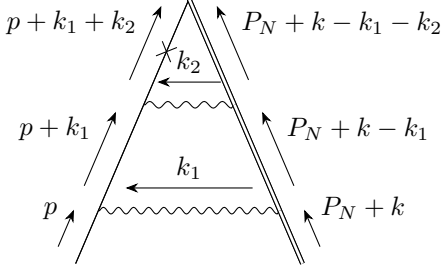
$$\begin{aligned}
&= -\mu^{2\epsilon} Z^2 e^4 \left[\int \frac{[dk_1]}{|\mathbf{k}_1|^2} \frac{[dk_2]}{|\mathbf{k}_2|^2} \frac{1}{k^0 - k_1^0 - k_2^0 + i\epsilon} \frac{1}{k^0 - k_1^0 + i\epsilon} \frac{(\mathbf{p} + \mathbf{k}_1)^4 / 8m^3}{\left[E + k_1^0 - \frac{(\mathbf{p} + \mathbf{k}_1)^2}{2m} + i\epsilon \right]^2} \frac{1}{E + k_1^0 + k_2^0 - \frac{(\mathbf{p} + \mathbf{k}_1 + \mathbf{k}_2)^2}{2m} + i\epsilon} \right] \\
&= 4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{|\mathbf{k}_1|^4 / 4m^2}{[|\mathbf{k}_1|^2 - 2mE']^2} \frac{1}{|\mathbf{k}_2|^2 - 2mE'}
\end{aligned}$$

after integrated \mathbf{k}_2 , the integral becomes

$$\begin{aligned}
&= 4m^2 \mu^{2\epsilon} \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{|\mathbf{k}_1|^4 / 4m^2}{[|\mathbf{k}_1|^2 - 2mE']^2} \frac{1}{\left(\mathbf{k}_1^2 - \frac{2mE'}{x_1} \right)^{2-d/2}} \left[\alpha^2 2^{4-d} \pi^{2-\frac{d}{2}} Z^2 \Gamma\left(2 - \frac{d}{2}\right) (x_1 - x_1^2)^{\frac{d}{2}-2} \right] \\
&= Z^2 \alpha^2 \mu^{2\epsilon} \int_0^1 dx_1 dx_2 dy_1 dy_2 dy_3 \delta(x_1 + x_2 - 1) \delta(y_1 + y_2 + y_3 - 1) \\
&\quad \left\{ 2^{4-2d} \pi^{2-d} p^4 y_1^4 y_2 (x_1 - x_1^2)^{\frac{d}{2}-2} y_3^{1-\frac{d}{2}} \Gamma(5-d) \left(\frac{1}{\frac{2E' m x_2 y_3}{(x_1-1)x_1} - 2E' m y_2 + p^2 (-y_1^2) + p^2 y_1} \right)^{5-d} \right. \\
&\quad + \frac{2^{5-2d} \pi^{2-d} p^2 y_1^2 y_2 (x_1 - x_1^2)^{\frac{d}{2}-2} y_3^{1-\frac{d}{2}} \Gamma(4-d) \Gamma\left(\frac{d}{2} + 1\right)}{\Gamma\left(\frac{d}{2}\right)} \left(\frac{1}{\frac{2E' m x_2 y_3}{(x_1-1)x_1} - 2E' m y_2 + p^2 (-y_1^2) + p^2 y_1} \right)^{4-d} \\
&\quad + \frac{2^{6-2d} \pi^{2-d} p^2 y_1^2 y_2 (x_1 - x_1^2)^{\frac{d}{2}-2} y_3^{1-\frac{d}{2}} \Gamma(4-d) \Gamma\left(\frac{d}{2} + 1\right)}{\Gamma\left(\frac{d}{2}\right) d} \left(\frac{1}{\frac{2E' m x_2 y_3}{(x_1-1)x_1} - 2E' m y_2 + p^2 (-y_1^2) + p^2 y_1} \right)^{4-d} \\
&\quad \left. + \frac{2^{4-2d} \pi^{2-d} y_2 (x_1 - x_1^2)^{\frac{d}{2}-2} y_3^{1-\frac{d}{2}} \Gamma(3-d) \Gamma\left(\frac{d}{2} + 2\right)}{\Gamma\left(\frac{d}{2}\right)} \left(\frac{1}{\frac{2E' m x_2 y_3}{(x_1-1)x_1} - 2E' m y_2 + p^2 (-y_1^2) + p^2 y_1} \right)^{3-d} \right\}
\end{aligned}$$

finish the integration of Feynman parameters, we have

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



$$\begin{aligned}
&= -\mu^{2\epsilon} Z^2 e^4 \left[\int \frac{[dk_1]}{|\mathbf{k}_1|^2} \frac{[dk_2]}{|\mathbf{k}_2|^2} \frac{1}{k^0 - k_1^0 - k_2^0 + i\epsilon} \frac{1}{k^0 - k_1^0 + i\epsilon} \frac{1}{E + k_1^0 - \frac{(\mathbf{p}+\mathbf{k}_1)^2}{2m} + i\epsilon} \frac{(\mathbf{p}+\mathbf{k}_2)^4/8m^3}{\left[E + k_1^0 + k_2^0 - \frac{(\mathbf{p}+\mathbf{k}_1+\mathbf{k}_2)^2}{2m} + i\epsilon \right]^2} \right] \\
&= 4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE'} \frac{|\mathbf{k}_2|^4/4m^2}{[|\mathbf{k}_2|^2 - 2mE']^2} \\
&= \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE'} \left\{ 1 + \frac{4mE'}{|\mathbf{k}_2|^2 - 2mE'} + \frac{(2mE')^2}{[|\mathbf{k}_2|^2 - 2mE']^2} \right\}
\end{aligned}$$

only the highest order of \mathbf{k}_2 in the polynomial can contribute to the divergence, other terms are finite and can be dropped in the following calculations. This can be observed by simply counting the superficial divergence. Then one could find that by shifting \mathbf{k}_2 this integral becomes scaleless, thus zero under dimensional regularization

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

We can see that the total divergence is

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

Comparing the final result of divergence between OPE and QM wavefunctions, we can see that the coefficient of $\log \mu$ is consistent with which of the logarithm divergence in the asymptotic behavior of Klein-Gordon wavefunction and Schrödinger wavefunction with relativistic correction.

4 Operator Product Expansion and Explicitly Coordinate-dependent Divergence

Now that we have successfully isolated the logarithmic divergence of local operators, we can calculate the coordinate-dependent divergence that we actually encountered regarding the wavefunction. As mentioned before, we can achieve that via OPE.

The operator product expansion [7] (OPE) is to write the products of several local operators evaluated at different points, in the limit of those points approaching each other, as a series of composite local operators, i.e.

$$\mathcal{O}_1(x) \mathcal{O}_2(y) = \sum_n C_n(x-y) \mathcal{O}_n(x) \quad (35)$$

In our case, the equation becomes

$$\psi(x) N(0) = C_0(x) \psi(0) N(0) + \sum_n C_n(x) \mathcal{O}_n(0) \quad (36)$$

The logarithmic divergence, which is the highest order of divergence on the left hand side, only appears in the coefficient of the first term in the right hand side. Since it's an equation for operators, we can also write it down as matrix elements

$$\langle 0|\psi(x)N(0)|0\rangle = C_0(x)\psi(0)N(0) + \sum_n C_n(x)\mathcal{O}_n(0) \quad (37)$$

The matrix element $\langle 0|\psi(0)N(0)|0\rangle$, is exactly what we calculated in the last section.

For any type of diagrams on the left hand side of equation (37), we have

$$\begin{array}{c} x \quad 0 \\ \text{Diagram} \end{array} = \left[\begin{array}{c} \text{Diagram} \\ p \quad P_N \end{array} \right] - UV + \left[\begin{array}{c} x \quad 0 \\ \text{Diagram} \\ p \quad P_N \end{array} \right] - \left[\begin{array}{c} \text{Diagram} \\ p \quad P_N \end{array} \right] + UV \quad (38)$$

where UV stands for the ultraviolet divergent part in the local matrix elements. So by using our previous results, we only have to compute the second term, which is in fact a Fourier transformation.

In previous discussion, we mentioned that the small distance between two field operators in OPE can be treated as a regularization scheme, so we can safely assume that only OPE diagrams correspondent with logarithmic divergent local operator diagrams contains $\log x$ terms. Therefore, in this case, only one diagram is considered. Here we'll jump to the 3-dimension integral without temporal component (for details about involved contour integral, see Appendix B).

$$\begin{aligned} & \begin{array}{c} x \quad 0 \\ \text{Diagram} \end{array} - \begin{array}{c} \text{Diagram} \end{array} \\ &= 4m^2\mu^{2\epsilon}Z^2e^4 \int \frac{d^d\mathbf{k}_1}{(2\pi)^d} \frac{d^d\mathbf{k}_2}{(2\pi)^d} [e^{-i\mathbf{k}_2\cdot\mathbf{x}} - 1] \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{|\mathbf{k}_1|^4/4m^2}{[|\mathbf{k}_1|^2 - 2mE']^2} \frac{1}{|\mathbf{k}_2|^2 - 2mE'} \\ &= 4m^2\mu^{2\epsilon}Z^2e^4 \int_0^1 dx_1 dx_2 dx_3 \delta(1 - x_1 - x_2 - x_3) \int \frac{d^d\mathbf{k}_2}{(2\pi)^d} [e^{-i\mathbf{k}_2\cdot\mathbf{x}} - 1] \frac{1}{|\mathbf{k}_2|^2 - 2mE'} \\ & \quad \frac{3x_3 (\mathbf{k}_2^4 x_2^4 + 2\mathbf{k}_2^2 \mathbf{p}^2 x_2^2 x_1^2 + 4\mathbf{k}_2^2 x_2^3 x_1 \mathbf{k}_2 \cdot \mathbf{p} + 4\mathbf{p}^2 x_2 x_1^3 \mathbf{k}_2 \cdot \mathbf{p} + 4x_2^2 x_1^2 (\mathbf{k}_2 \cdot \mathbf{p})^2 + \mathbf{p}^4 x_1^4)}{32\pi} \\ & \quad \left(\frac{1}{\mathbf{k}_2^2 x_2 - (-\mathbf{k}_2 x_2 - \mathbf{p} x_1)^2 - 2Emx_3 + \mathbf{p}^2 x_1} \right)^{5/2} + \frac{3x_3 (\frac{10}{3}\mathbf{k}_2^2 x_2^2 + \frac{20}{3}x_2 x_1 \mathbf{k}_2 \cdot \mathbf{p} + \frac{10}{3}\mathbf{p}^2 x_1^2)}{32\pi} \\ & \quad \left(\frac{1}{\mathbf{k}_2^2 x_2 - (-\mathbf{k}_2 x_2 - \mathbf{p} x_1)^2 - 2Emx_3 + \mathbf{p}^2 x_1} \right)^{3/2} + \frac{15x_3}{32\pi} \sqrt{\frac{1}{\mathbf{k}_2^2 x_2 - (-\mathbf{k}_2 x_2 - \mathbf{p} x_1)^2 - 2Emx_3 + \mathbf{p}^2 x_1}} \end{aligned} \quad (39)$$

Appendices

A Useful formulas in Feynman integrals

Feynman parametrization used here is

$$\frac{1}{\prod A_i^{d_i}} = \int \prod dx_i \delta(\sum x_i - 1) \frac{\prod x_i^{d_i-1}}{[\sum x_i A_i]^{\sum d_i}} \frac{\Gamma(\sum d_i)}{\prod \Gamma(d_i)} \quad (40)$$

Schwinger parametrization will also be useful

$$\frac{1}{A^n} = \frac{1}{\Gamma(n)} \int_0^\infty dz z^{n-1} e^{-zA} \quad (41)$$

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

$$\int \frac{d^d k}{(2\pi)^d} \frac{k^{2\beta}}{(k^2 + \Delta)^n} = \frac{1}{(4\pi)^{n-\beta}} \frac{\Gamma(\beta + d/2)}{\Gamma(d/2)} \frac{\Gamma(n - \beta - d/2)}{\Gamma(n)} \left(\frac{4\pi}{\Delta}\right)^{n-\beta-d/2} \quad (42a)$$

$$= \frac{1}{(4\pi)^{d/2}} \frac{\Gamma(\beta + d/2)}{\Gamma(d/2)} \frac{\Gamma(n - \beta - d/2)}{\Gamma(n)} \left(\frac{1}{\Delta}\right)^{n-\beta-d/2} \quad (42b)$$

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

B Contour Integral

If the nucleus is put on-shell, integral with the structure of the form

$$\int [dk_1][dk_2] f(\mathbf{k}_1, \mathbf{k}_2) \frac{1}{-k_1^0 - k_2^0 + i\epsilon} \frac{1}{-k_1^0 + i\epsilon} \frac{1}{[E + k_1^0 - \mathbf{V}_2 + i\epsilon]^m} \frac{1}{[E + k_1^0 + k_2^0 - \mathbf{V}_2 + i\epsilon]^n} \quad (43)$$

will always produce

$$\int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} f(\mathbf{k}_1, \mathbf{k}_2) \frac{1}{[E - \mathbf{V}_1 + 2i\epsilon]^m} \frac{1}{[E - \mathbf{V}_2 + 2i\epsilon]^n} \quad (44)$$

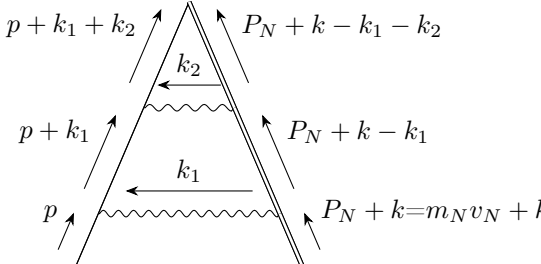
with k_1^0 and k_2^0 goes to zero.

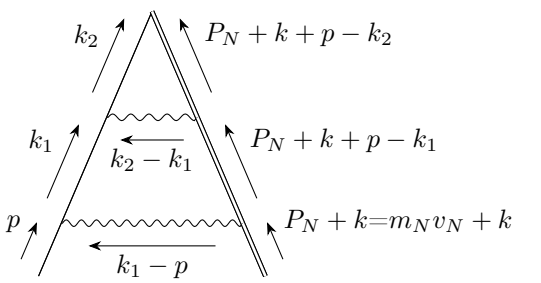
If the nucleus is slightly off-shell by k , there'll be a slight shift of energy in the non-relativistic propagators

$$\begin{aligned} & \int [dk_1][dk_2] f(\mathbf{k}_1, \mathbf{k}_2) \frac{1}{-k_1^0 - k_2^0 + k^0 + i\epsilon} \frac{1}{-k_1^0 + k^0 + i\epsilon} \frac{1}{[E + k_1^0 - \mathbf{V}_2 + i\epsilon]^m} \frac{1}{[E + k_1^0 + k_2^0 - \mathbf{V}_2 + i\epsilon]^n} \\ &= \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} f(\mathbf{k}_1, \mathbf{k}_2) \frac{1}{[E + k^0 - \mathbf{V}_1 + 2i\epsilon]^m} \frac{1}{[E + k^0 - \mathbf{V}_2 + 2i\epsilon]^n} \end{aligned}$$

If we define $E' = E + k^0$, the structure falls back to (44).

One example is this Green function

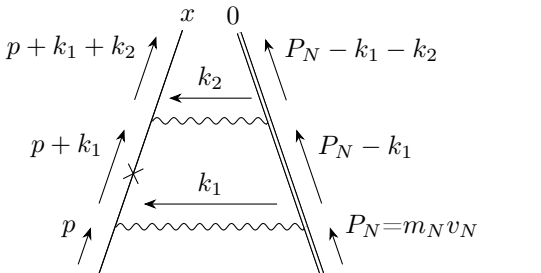


$$\begin{aligned}
&= -\mu^{2\epsilon} Z^2 e^4 \left[\int \frac{[dk_1]}{|\mathbf{k}_1|^2} \frac{[dk_2]}{|\mathbf{k}_2|^2} \frac{1}{k^0 - k_1^0 - k_2^0 + i\epsilon} \frac{1}{k^0 - k_1^0 + i\epsilon} \frac{1}{E + k_1^0 - \frac{(\mathbf{p}+\mathbf{k}_1)^2}{2m} + i\epsilon} \frac{1}{E + k_1^0 + k_2^0 - \frac{(\mathbf{p}+\mathbf{k}_1+\mathbf{k}_2)^2}{2m}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


$$= \text{Diagram with shifted momenta}$$

As for any OPE diagram, it's just a regular local one multiplied by a exponential factor, and since we're choosing $x = (0, \mathbf{x})$, this factor can be included into $f(\mathbf{k}_1, \mathbf{k}_2)$ in (43). That means it also becomes (44). We also performed a momentum shift in the computation of regular local ones, what we did is basically assign \mathbf{k}_2 to the upper photon line and after the contour integral, we reassign \mathbf{k}_2 to the upper electron line. Therefore the exponential factor will always becomes $e^{-i\mathbf{k}_2 \cdot \mathbf{x}}$ in the end.

For example,



$$\begin{aligned}
&= -\mu^{2\epsilon} Z^2 e^4 \left[\int \frac{[dk_1]}{|\mathbf{k}_1|^2} \frac{[dk_2]}{|\mathbf{k}_2|^2} \frac{e^{-i(\mathbf{p}+\mathbf{k}_1+\mathbf{k}_2) \cdot \mathbf{x}}}{k^0 - k_1^0 - k_2^0 + i\epsilon} \frac{1}{k^0 - k_1^0 + i\epsilon} \frac{(\mathbf{p} + \mathbf{k}_1)^4 / 8m^3}{\left[E + k_1^0 - \frac{(\mathbf{p}+\mathbf{k}_1)^2}{2m} + i\epsilon \right]^2} \frac{1}{E + k_1^0 + k_2^0 - \frac{(\mathbf{p}+\mathbf{k}_1+\mathbf{k}_2)^2}{2m} + i\epsilon} \right] \\
&= \mu^{2\epsilon} Z^2 e^4 \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} e^{-i(\mathbf{p}+\mathbf{k}_1+\mathbf{k}_2) \cdot \mathbf{x}} \frac{1}{|\mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_2|^2} \frac{(\mathbf{p} + \mathbf{k}_1)^4 / 8m^3}{\left[E' - \frac{(\mathbf{p}+\mathbf{k}_1)^2}{2m} + 2i\epsilon \right]^2} \frac{1}{E' - \frac{(\mathbf{p}+\mathbf{k}_1+\mathbf{k}_2)^2}{2m} + 2i\epsilon}
\end{aligned}$$

perform shifts $\mathbf{k}_1 \rightarrow \mathbf{k}_1 - \mathbf{p}$ and $\mathbf{k}_2 \rightarrow \mathbf{k}_2 - \mathbf{k}_1 - \mathbf{p}$

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

which is exactly the form in (39).

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