

Divergence of Klein-Gordon Hydrogen Wavefunction Near Origin

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Introduction

1 Divergence in Klein-Gordon Equation and Schrödinger Equation

1.1 Klein-Gordon Equation Solution

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

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

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

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

$$-(Z\alpha)^2 \log(mr) \quad (6)$$

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

1.2 The Schrödinger part

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

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

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

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

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

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

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

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

The NLO correction of the bound state wave function is

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

with

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

and

$$a_{k1} = \frac{2\alpha^4 e^{\frac{\pi}{2k}} k m^2 Z^4 |\Gamma(1 - \frac{i}{k})| \left(\alpha^2 k^2 m^2 Z^2 - 2\alpha^2 \left(1 - \frac{i}{k}\right)^{i/k} \left(1 + \frac{i}{k}\right)^{-\frac{i}{k}} m^2 Z^2 \cosh\left(\frac{\pi}{k}\right) + \alpha^2 m^2 Z^2 \right)}{(\alpha^2 k^2 m^2 Z^2 + \alpha^2 m^2 Z^2)^2}$$

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 and also a down-limit λ , with $\lambda \gg 1$ (note that the following wave function have been multiplied by $2(mZ\alpha)^{\frac{3}{2}}$)

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

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

$$\Phi^{(1)}(0)_{kin} = \int_{\lambda}^{\frac{\Lambda}{m}} dk (Z\alpha)^2 \left(\frac{1}{\pi} + \frac{1}{k}\right) \quad (14)$$

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

The UV divergent part of Darwin term is

$$\Phi^{(1)}(0)_D = -\frac{(Z\alpha)^4}{8\pi} \int_{\lambda}^{\frac{\Lambda}{m}} dk k^2 e^{\frac{\pi}{k}} |\Gamma(1 - \frac{i}{k})|^2 \quad (16)$$

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

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

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

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 perturbative Schrödinger wave function's origin UV divergence, with a k 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 Non-relativistic Scalar QED (NRSQED) Matching

2.1 Operator Product Expansion

In the following sections we work on the quantum field theory side. 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. For simplicity, there's no need involving any other effect the nucleus might have. Therefore, we can describe the wavefunction in terms of a matrix element $\langle 0|\psi(x)N(0)|0\rangle$. The divergence of this non-local matrix element can be analyzed by operator product expansion.

The operator product expansion (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.

$$\mathcal{O}_1(x)\mathcal{O}_2(y) = \sum_n C_n(x-y)\mathcal{O}_n(x) \quad (22)$$

In our case, the equation becomes

$$\langle 0|\psi(x)N(0)|0\rangle = \langle 0|C_0(x)\mathcal{O}_0(0) + \sum_n C_n(x)\mathcal{O}_n(0)|0\rangle \quad (23)$$

The logarithmic divergence, which is the highest order of divergence on the left hand side, only appears in the first term of the right hand side.

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 non-relativistic scalar QED 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.

2.2 Feynman Rules

2.2.1 Scalar QED (SQED)

The Lagrangian of scalar QED is

$$\mathcal{L}_{SQED} = |D_\mu\phi|^2 - m^2|\phi|^2 + \Phi_v^* i v \cdot D \Phi_v \quad (24)$$

with the covariant derivative defined as

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

and

$$D_\mu\Phi_v = \partial_\mu\Phi - iZeA_\mu\Phi_v$$

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

2.2.2 NRSQED

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

$$\mathcal{L}_{NRSQED} = \varphi^* \left(iD_0 + \frac{\mathbf{D}^2}{2m} \right) \varphi + \delta\mathcal{L} + \Phi_v^* i v \cdot D \Phi_v \quad (25)$$

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

$$\delta\mathcal{L} = \frac{(D_0\varphi)^*(D_0\varphi)}{2m} = \frac{\dot{\varphi}^*\dot{\varphi}}{2m} + \frac{e^2\varphi^*\varphi A_0^2}{2m} - \frac{ie}{2m}A_0(\varphi^*\dot{\varphi} - \dot{\varphi}^*\varphi) \quad (26)$$

and it changes the Feynman rules to¹

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

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).

2.2.3 NRSQED Lagrangian via HSET transformation

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

$$\mathcal{L}_{SQED} = |D_\mu \phi|^2 - m^2 |\phi|^2 \quad (27)$$

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

$$\varphi_v = \frac{1}{\sqrt{2m}} e^{imv \cdot x} (iv \cdot D + m) \phi \quad (28)$$

$$\bar{\varphi}_v = \frac{1}{\sqrt{2m}} e^{imv \cdot x} (-iv \cdot D + m) \phi \quad (29)$$

then

$$\mathcal{L}_{SQED} = \frac{1}{2m} (D_\mu (\varphi_v + \bar{\varphi}_v))^* D^\mu (\varphi_v + \bar{\varphi}_v) + (\varphi_v + \bar{\varphi}_v)^* iv \cdot D (\varphi + \bar{\varphi}_v) \quad (30)$$

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

$$\bar{\varphi}_v = \frac{-iD_0}{2m} (\varphi_v + \bar{\varphi}_v) \quad (31)$$

$$\frac{-iD_0}{2m} \varphi_v = \frac{\nabla^2}{4m^2} (\varphi_v + \bar{\varphi}_v) \quad (32)$$

And (27) could be transformed as

$$\mathcal{L}_{SQED} = (\varphi_v + \bar{\varphi}_v)^* (iD_0 + \frac{\nabla^2}{2m} - \frac{D_0^2}{2m}) (\varphi + \bar{\varphi}_v) \quad (33)$$

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

$$\mathcal{L}_{SQED} = \varphi_v^* (iD_0 + \frac{\nabla^2}{2m} + \frac{\nabla^4}{8m^3} + \frac{\nabla^6}{16m^5} + \frac{e}{32m^4} ([\nabla^2, [A_0, \nabla^2]] + [A_0, \nabla^4]) + \mathcal{O}(v^7)) \varphi_v \quad (34)$$

2.3 LO Matching

2.3.1 SQED

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


2.3.2 NRSQED

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

which gives

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

The new electron-photon vertex is



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

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 $1/32m^4$.

3 Local Operator and Matrix Element of NRSQED

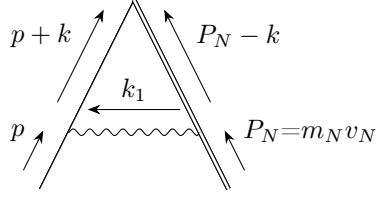
To reproduce the singular behavior of “Klein-Gordon Hydrogen” wavefunction near origin, we can try OPE. But the dependence of x in OPE can be taken as a regularization scheme and thus the result should be the same as local one without renormalization. And the logarithmic terms of x in OPE can be reproduced 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 NLO

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

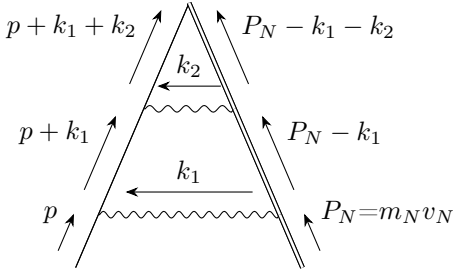
First we define $\epsilon = 3 - d$. After dimensional regularization, the Gamma function in the numerator is something like $\Gamma(n - d/2)$ and Gamma function doesn't have pole at half integer. We can prove that any one-loop diagram

involved does not have logarithmic divergence, for example

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


which doesn't have logarithm divergence.

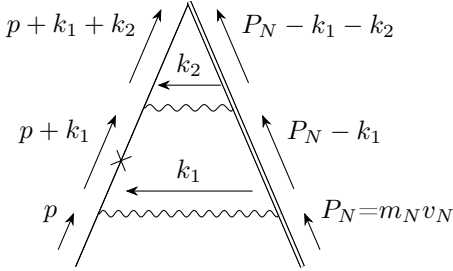
3.2 NNLO



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

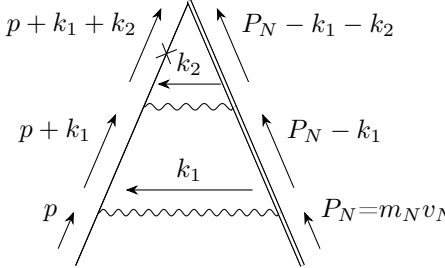
integrate out the temporal component of loop momentum, then perform a shift on them

$$= \mu^{2\epsilon} Z^2 e^4 \left[\int \frac{d^3 \mathbf{k}_1}{(2\pi)^3} \frac{d^3 \mathbf{k}_2}{(2\pi)^3} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{E - \frac{|\mathbf{k}_1|^2}{2m} + 2i\epsilon} \frac{1}{E - \frac{|\mathbf{k}_2|^2}{2m} + 2i\epsilon} \right] = 0$$



$$= 4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^3 \mathbf{k}_1}{(2\pi)^3} \frac{d^3 \mathbf{k}_2}{(2\pi)^3} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{|\mathbf{k}_1|^4 / 4m^2}{[|\mathbf{k}_1|^2 - 2mE]^2} \frac{1}{|\mathbf{k}_2|^2 - 2mE}$$

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



$$= 4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^3 \mathbf{k}_1}{(2\pi)^3} \frac{d^3 \mathbf{k}_2}{(2\pi)^3} \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_1|^2 - 2mE} \frac{|\mathbf{k}_2|^4/4m^2}{[|\mathbf{k}_2|^2 - 2mE]^2}$$

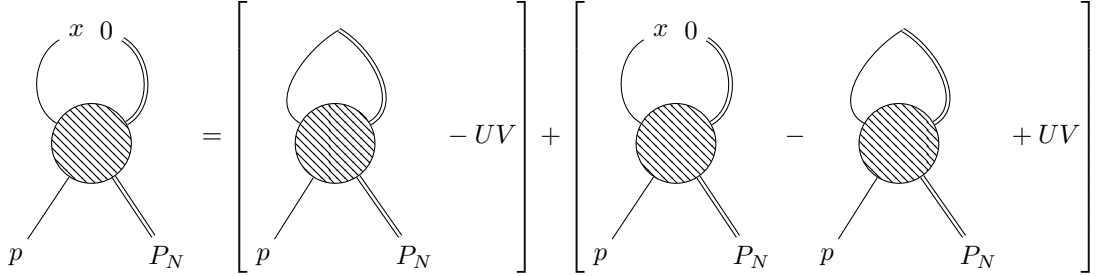
=0 + finite terms

we can see that the total divergence is $Z^2 \alpha^2 (\frac{1}{2(3-d)} + \log \mu)$.

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. For any type of diagrams on the left hand side of equation (23), we have

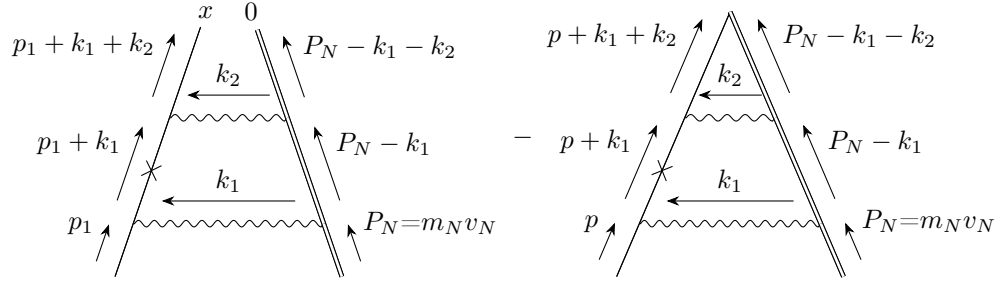


$$= \left[\text{diagram} - UV \right] + \left[\text{diagram} - \text{diagram} + UV \right] \quad (35)$$

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.



$$= 4m^2 \mu^{2\epsilon} Z^2 e^4 \int \frac{d^3 \mathbf{k}_1}{(2\pi)^3} \frac{d^3 \mathbf{k}_2}{(2\pi)^3} [e^{-i\mathbf{k}_2 \cdot \mathbf{x}} - 1] \frac{1}{|\mathbf{k}_1 - \mathbf{p}|^2} \frac{1}{|\mathbf{k}_2 - \mathbf{k}_1|^2} \frac{|\mathbf{k}_1|^4 / 4m^2}{[|\mathbf{k}_1|^2 - 2mE]^2} \frac{1}{|\mathbf{k}_2|^2 - 2mE}$$

Appendices

A Useful formulas in Feynman integrals

Feynman parametrization used here is

$$\frac{1}{\prod A_i^{d_i}} = \int \prod dx_i \delta(\sum x_i - 1) \frac{\prod x_i^{d_i-1}}{[\sum x_i A_i]^{\sum d_i}} \frac{\Gamma(\sum d_i)}{\prod \Gamma(d_i)} \quad (36)$$

Schwinger parametrization will also be useful

$$\frac{1}{A^n} = \frac{1}{\Gamma(n)} \int_0^\infty dz z^{n-1} e^{-zA} \quad (37)$$

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

$$\int \frac{d^3\mathbf{k}_1}{(2\pi)^3} \frac{d^3\mathbf{k}_2}{(2\pi)^3} \frac{1}{|\mathbf{k}_1|^2} \frac{1}{|\mathbf{k}_2|^2} \frac{1}{[p^0 - M - \frac{(\mathbf{p}+\mathbf{k}_1)^2}{2M}]^m} \frac{1}{[p^0 - M - \frac{(\mathbf{p}+\mathbf{k}_1+\mathbf{k}_2)^2}{2M} + i\epsilon]^n}$$

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

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

$$\int \frac{d^d k}{(2\pi)^d} \frac{k^{2\beta}}{(k^2 + \Delta)^n} = \frac{1}{(4\pi)^{n-\beta}} \frac{\Gamma(\beta + d/2)}{\Gamma(d/2)} \frac{\Gamma(n - \beta - d/2)}{\Gamma(n)} \left(\frac{4\pi}{\Delta}\right)^{n-\beta-d/2} \quad (38a)$$

$$= \frac{1}{(4\pi)^{d/2}} \frac{\Gamma(\beta + d/2)}{\Gamma(d/2)} \frac{\Gamma(n - \beta - d/2)}{\Gamma(n)} \left(\frac{1}{\Delta}\right)^{n-\beta-d/2} \quad (38b)$$

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

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