IFT, Madrid

Frontiers in Lattice Quantum Field Theory

QCD+QED and numerical simulations

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- Motivations and general introduction
- Charged states in finite volume
- Gauge-invariant charged states
- Crash intro to decay rates

Introduction

Motivations and general introduction

Motivations

- In the real world up and down quarks have different masses and electric charges.

- Isospin-breaking effects are typically a few percent effects:

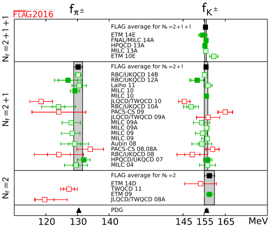
$$\frac{m_u - m_d}{M_p} \simeq 0.3\% \qquad \alpha_{\text{EM}} = 0.7\% \qquad \frac{M_n - M_p}{M_n} \simeq 0.1\%$$

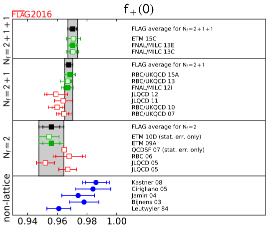
- From FLAG16 [Aoki *et al.*, arXiv:1607.00299] and [PDG review, Rosner *et al.*, 2016], [Cirigliano *et al.*, Rev. Mod. Phys. **84**, 399 (2012)]

$$f_{\pi^\pm} = 130.2(1.4)\ \text{MeV} \qquad \text{err} = 1\% \qquad \delta^{\chi\text{PT}}_{\text{QED}}(\pi^- \to \ell^- \bar{\nu}) = 1.8\%$$

$$f_{K^\pm} = 155.6(0.4)\ \text{MeV} \qquad \text{err} = 0.3\% \qquad \delta^{\chi\text{PT}}_{\text{QED}}(K^- \to \ell^- \bar{\nu}) = 1.1\%$$

$$f_+(0) = 0.9704(24)(22) \qquad \text{err} = 0.5\% \qquad \delta^{\chi\text{PT}}_{\text{QED}}(K \to \pi \ell \bar{\nu}) = [0.5, 3]\%$$





Two ways for QCD+QED on the lattice

- Expand observables with respect to α_{em} and Δm_{ud} analytically, and calculate the coefficients of the expasion by simulating QCD only.

  de Divitiis *et al.* (RM123), Leading isospin breaking effects on the lattice, Phys.Rev. D87 (2013) 11, 114505.

- Simulate QCD+QED on the lattice, typically at a larger value of α_{em} and Δm_{ud} and extrapolate to physical values.

  Borsanyi *et al.*, Ab initio calculation of the neutron-proton mass difference, Science 347 (2015) 1452-1455.

Sketching the RM123 method

QCD+QED action, assume only u and d for simplicity

$$S_{\mathrm{Q[C+E]D}} = \int_x \left\{ \frac{1}{4g_0^2} \mathrm{tr}\, G^2 + \frac{1}{4} F^2 + \sum_{f=u,d} \bar{\psi}_f [\not{D} + m_0^f] \psi_f + i e_0 A_\mu j_\mu \right\}$$

$$D_\mu = \partial_\mu + i B_\mu \qquad\qquad j_\mu = \sum_{f=u,d} q_f \bar{\psi}_f \gamma_\mu \psi_f$$

Physical observables can be expanded in powers of (the renormalized) α_{em} and Δm^{ud}. Notice that the bare parameters depend on α_{em} and Δm^{ud} through the renormalization conditions, e.g. $g_0^2 = g_0^2(\alpha_{em}, \Delta m^{ud})$.

$$e^{-S_{\mathrm{Q[C+E]D}}} = e^{-S_{\mathrm{iso}}} \Bigg\{ 1 - i e_0 \int_x A_\mu(x) j_\mu(x) - \int_x \left[\frac{c_0}{4} \mathrm{tr}\, G^2(x) + \sum_{f=u,d} \Delta m_0^f \bar{\psi}_f \psi_f(x) \right] + \\ + \frac{e_0^2}{2} \int_{xy} A_\mu(x) j_\mu(x) A_\nu(y) j_\nu(y) + O(\alpha_{em}^{3/2}) + O(\Delta m_{ud}^2) \Bigg\}$$

Sketching the RM123 method

$$e^{-S_{\mathrm{Q[C+E]D}}} = e^{-S_{\mathrm{iso}}} \Big\{ 1 - ie_0 \int_x A_\mu(x) j_\mu(x) - \int_x \left[\frac{c_0}{4} \mathrm{tr}\, G^2(x) + \sum_{f=u,d} \Delta m_0^f \bar{\psi}_f \psi_f(x) \right] + \\ + \frac{e_0^2}{2} \int_{xy} A_\mu(x) j_\mu(x) A_\nu(y) j_\nu(y) + O(\alpha_{em}^{3/2}) + O(\Delta m_{ud}^2) \Big\}$$

If P is an observable that does not depend on the photon field

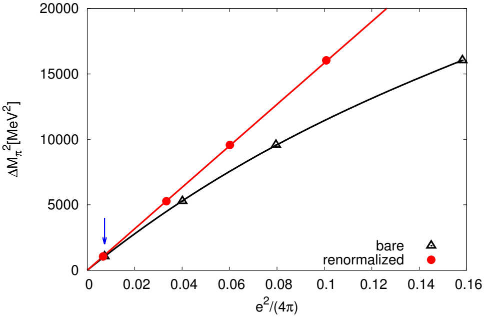
$$\langle P \rangle_{\mathrm{Q[C+E]D}} = \langle P \rangle_{\mathrm{iso}} - \int_x \langle \left[\frac{c_0}{4} \mathrm{tr}\, G^2(x) + \sum_{f=u,d} \Delta m_0^f \bar{\psi}_f \psi_f(x) \right] P \rangle_{0,c} + \\ + \frac{e_0^2}{2} \int_{xy} \Delta_{\mu\nu}(x-y) \langle j_\mu(x) j_\nu(y) P \rangle_{0,c} + \ldots$$

If P transforms non-trivially under isospin rotations

$$\langle P \rangle_{\mathrm{Q[C+E]D}} = -\frac{\Delta m_0^{ud}}{2} \int_x \langle [\bar{\psi}_u \psi_u(x) - \bar{\psi}_d \psi_d(x)] P \rangle_{0,c} + \\ + \frac{e_0^2}{2} \int_{xy} \Delta_{\mu\nu}(x-y) \langle j_\mu(x) j_\nu(y) P \rangle_{0,c} + \ldots$$

Sketching the BMW method

Simulate the full QCD+QED theory on the lattice. Since isospin-breaking effect are small, one needs to amplify them by simulating at larger values of α_{em} and Δm_{ud}. An interpolation is needed.



Two ways for QCD+QED on the lattice

- RM123 method

$$\langle P\rangle_{\mathrm{Q[C+E]D}} = -\frac{\Delta m_0^{ud}}{2}\int_x \langle[\bar\psi_u\psi_u(x)-\bar\psi_d\psi_d(x)]P\rangle_{0,c}+ \\ +\frac{e_0^2}{2}\int_{xy}\Delta_{\mu\nu}(x-y)\langle j_\mu(x)j_\nu(y)P\rangle_{0,c}+\dots$$

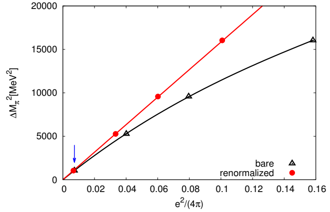
Pros:
Only $O(\alpha_{em}^0)$ observables.

Cons:
Complex observables (e.g. a 4-point functions for mass correction), typically involving fermionic disconnected diagrams.

- BMW method

Pros:
Simpler observables (e.g. 2-point functions for mass correction).

Cons:
Signal is typically $O(\alpha_{em})$.



Charged states in finite volume

Quick review of methods you'll hear about here

Charge states in a finite box

In a finite box with periodic boundary conditions, Gauss law forbids states with nonzero charge

$$Q = \int \mathrm{d}^3x \; j_0(t, \mathbf{x}) = \int \mathrm{d}^3x \; \partial_k E_k(t, \mathbf{x}) = 0$$

QED + Feynman gauge $\quad\Rightarrow\quad$ electron two-point function $\langle \psi(x) \bar{\psi}(y) \rangle$
However in finite volume, large gauge transformations *survive* a local gauge fixing

$$A_\mu(x) \to A_\mu(x) + \frac{2\pi n_\mu}{L} \; , \quad \psi(x) \to e^{\frac{2\pi i n_\mu x_\mu}{L}} \psi(x)$$

$$\langle \psi(x) \bar{\psi}(y) \rangle \to e^{\frac{2\pi i n_\mu (x-y)_\mu}{L}} \langle \psi(x) \bar{\psi}(y) \rangle \qquad \Rightarrow \qquad \langle \psi(x) \bar{\psi}(y) \rangle = 0$$

Large gauge transformations shift the zero-modes of the photon field.

- Various constraints on some momentum components of the photon field. Hayakawa, Uno, Prog. Theor. Phys. 120 (2008) 413-441.

  $$\int d^3x \; A_\mu(t, \mathbf{x}) = 0$$

  Widely used, but the constraint is non-local.

- Add a mass to the photon. Endres *et al.*, Phys. Rev. Lett. 117 (2016) no.7, 072002..
- Make the photon field antiperiodic (the only translational-invariant way to do this is by means of $C^\star$ boundary conditions). Wiese, Nucl. Phys. B 375, 45 (1992). Lucini *et al.*, JHEP 1602, 076 (2016).

$\mathrm{QED_L}$: spatial zero-modes

Hayakawa and Uno, Prog. Theor. Phys. **120**, 413 (2008)

Recipe: Remove the spatial zero-mode of the gauge field in each timeslice

$$\int \mathrm{d}^3x \; A_\mu(t,\mathbf{x}) = 0$$

$\mathrm{QED_L}$ has a transfer matrix. It is a nonlocal prescription. Locality is a core property of QFT, it is a fundamental assumption behind

- Renormalizability by power counting
- Volume-independence of renormalization constants
- Operator product expansion $\longrightarrow$ it fails for operators with enough large dimension
- Effective-theory description of long-distance physics $\longrightarrow$ it fails at large enough order
- Symanzik improvement program $\longrightarrow$ it fails at large enough order
- ...

Argument by N. Tantalo. Correction to the mass (Cotthingham formula)

$$\Delta m = \langle h|\mathrm{C.T.}|h\rangle_{c,QCD} - \frac{e^2}{4mL^3}\sum_{\mathbf{k}}\int \frac{dk_0}{2\pi}\,\frac{1-\delta_{\mathbf{k},\mathbf{0}}}{k^2}\int_{\mathbb{R}\times L^3} d^4x\; e^{-ikx}\langle h|\mathrm{T}\{j_\mu(x)j_\mu(0)\}|h\rangle_{c,QCD}$$

Large k_0-behaviour of the subtraction

$$\frac{1}{L^3}\int_{k_0<a^{-1}}\frac{dk_0}{2\pi}\,\frac{\delta_{\mathbf{k},\mathbf{0}}}{k_0^2}\,\frac{O_4}{k^2} = \frac{O_4\delta_{\mathbf{k},\mathbf{0}}}{L^3}\int_{k_0<a^{-1}}\frac{dk_0}{2\pi}\,\frac{1}{k_0^4} = \text{finite part} + \frac{a^3}{L^3}$$

Odd powers of a that are not chirally-suppressed, even in chirality-preserving discretizations.

$\mathrm{QED_m}$: massive photon

Endres *et al.*, arXiv:1507.08916

Recipe: Feynman gauge + mass term for photon.

Local prescription. Gauge invariance is broken in a controlled way (soflty broken). Infinite-volume limit must be taken before the $m_\gamma \to 0$ limit.

In the $m_\gamma \to 0$ limit

$$\langle \psi(x)\bar{\psi}(0)\rangle \propto e^{-\frac{e^2}{2m_\gamma^2 V}x_0^2} \langle \delta_{Q(T),0}\psi(x)\bar{\psi}(0)\rangle_{\mathrm{TL}}$$

where $\langle \cdot \rangle_0$ is the expectation value in $\mathrm{QED_{TL}}$. In this regime, $\mathrm{QED_m}$ is just a complicated way to calculate $\mathrm{QED_{TL}}$ expectation values.

The $e^{-x_0^2}$ is at odds with a standard transfer-matrix interpretation. The $\mathrm{QED_m}$ Hamiltonian is **not Hermitean**. Roughly speaking, the $e^{-x_0^2}$ is generated by a continuous Gaussian spectral density and imaginary eigenvalues of the Hamiltonian

$$\int dE \; e^{-E^2} e^{iEx_0} = e^{-x_0^2}$$

The Hamiltonian is Hermitean when restricted to the zero-charge sector (no funny behaviour), e.g. in the calculation of isospin-breaking corrections to the HVP.

C* boundary conditions

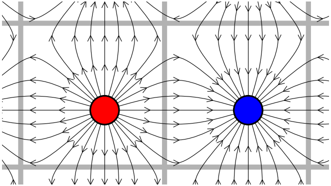
Wiese, Nucl. Phys. B **375**, 45 (1992)
Polley, Z. Phys. C **59**, 105 (1993)
Kronfeld and Wiese, Nucl. Phys. B **357**, 521 (1991)
Lucini, AP, Ramos, Tantalo, JHEP **1602**, 076 (2016)

Recipe: Use C* boundary conditions along spatial directions for all fields

$$A_\mu(x + L\mathbf{k}) = -A^*_\mu(x)$$
$$\psi(x + L\mathbf{k}) = C^{-1}\bar{\psi}^T(x)$$

The flux of electric fiels across the boundaries in not forced to vanish

$$Q(t) = \int \mathrm{d}^3x\, j_0(t, \mathbf{x}) = \int \mathrm{d}^3x\, \partial_k E_k(t, \mathbf{x}) \neq 0$$



Local prescription. Gauge invariance is preserved. Continuum limit can be consistently take *before* infinite-volume limit. Flavour and charge conservation are partially violated.

- This generates unphysical decay of a few hadrons, but most of them are protected. In n-point functions involving the non-protected hadrons, infinite-volume limit must be taken before the large-t limit.
- Non-physical decay is exponentially suppressed with the volume.
- Flavour symmetry is broken only by boundary effects. Composite operators renormalize as if flavour symmetry were intact.

Gauge-invariant charged states

Some exploratory runs

Interpolating operators for electrically-charged states

- In infinite volume it is possible to define gauge-invariant interpolating operators for charged states. These operators must be non-local, however they can be chosen to be local in time.
- Why do we care? Gauge fixing is perfectly fine in QED.

Interpolating operators for electrically-charged states

- In infinite volume it is possible to define gauge-invariant interpolating operators for charged states. These operators must be non-local, however they can be chosen to be local in time.
- Why do we care? Gauge fixing is perfectly fine in QED.
- In covariant gauge the Hilbert space includes non physical states, that need to be projected out by hand. In the Euclidean, the Hamiltonian is not hermitean. It is possible to write an effective Hamiltonian for the physical states. In the sector with non-zero charge, the effective Hamiltonian is time-dependent: physical states couple to an external, unphysical and time-dependent current.
- In gauge-invariant quantization, the Hilbert space contains only positive-norm state. Physical states are selected by requiring gauge invariance, i.e. they are automatically generated by gauge-invariant operators.

Interpolating operators for electrically-charged states

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- In gauge-invariant quantization, the Hilbert space contains only positive-norm state. Physical states are selected by requiring gauge invariance, i.e. they are automatically generated by gauge-invariant operators.
- With minimal effort, we can construct gauge-invariant interpolating operators for charged states. So why should we bother to fix the gauge?

Interpolating operators for electrically-charged states

- Dirac interpolating operator in infinite volume:

$$\Psi(t,\mathbf{x}) = e^{-\imath \int d^3y \ \Phi(\mathbf{y}-\mathbf{x})\partial_k A_k(t,\mathbf{y})}\psi(t,\mathbf{x})$$

where $\Phi(\mathbf{x})$ is the electric potential of a unit charge

$$\partial_k\partial_k\Phi(\mathbf{x}) = \delta^3(\mathbf{x})$$

- $\Psi(t,\mathbf{x})$ is invariant under infinitesimal gauge transformations with a compact support

$$A_k(t,\mathbf{x}) \to A_k(t,\mathbf{x}) + \partial_k\lambda(t,\mathbf{x}) \qquad \psi(t,\mathbf{x}) \to e^{\imath\lambda(t,\mathbf{x})}\psi(t,\mathbf{x})$$

$$e^{-\imath \int d^3y \ \Phi(\mathbf{y}-\mathbf{x})\partial_k A_k(t,\mathbf{y})} \to e^{-\imath \int d^3y \ \Phi(\mathbf{y}-\mathbf{x})\partial_k A_k(t,\mathbf{y})} e^{-\imath \int d^3y \ \Phi(\mathbf{y}-\mathbf{x})\partial_k \partial_k \lambda(t,\mathbf{y})} =$$

$$= e^{-\imath \int d^3y \ \Phi(\mathbf{y}-\mathbf{x})\partial_k A_k(t,\mathbf{y})} e^{-\imath\lambda(t,\mathbf{x})}$$

- $\Psi(t,\mathbf{x})$ is charged under global gauge transformations

$$A_k(t,\mathbf{x}) \to A_k(t,\mathbf{x}) \qquad \psi(t,\mathbf{x}) \to e^{i\alpha}\psi(t,\mathbf{x})$$

Interpolating operators for electrically-charged states

The Dirac interpolating operator can be constructed also in finite volume

$$\Psi(t,\mathbf{x}) = e^{-\imath \int d^3y \;\; \Phi(\mathbf{y}-\mathbf{x}) \partial_k A_k(t,\mathbf{y})} \psi(t,\mathbf{x})$$

provided that the Poisson equation has solutions

$$\partial_k \partial_k \Phi(\mathbf{x}) = \delta^3(\mathbf{x})$$

The Poisson equation has no solutions on a torus with peridic boundary conditions, while it admits a unique solution with C-parity boundary conditions

$$\Phi(\mathbf{x} + L\mathbf{k}) = -\Phi(\mathbf{x})$$

This construction is not unique!

Interpolating operators in the compact formulation

Lucini, AP, Ramos, Tantalo, JHEP **1602**, 076 (2016)
Hansen, Lucini, AP, Tantalo, JHEP xywz (2018)

- In the compact formulation the path-integral is well defined without gauge fixing

- Choose an unconventional normalization for the U(1) gauge field (action)

$$S = \frac{1}{g_0^2} \sum_{x,\mu\nu} \{1 - V_{\mu\nu}(x)\} + \frac{6^2}{2e_0^2} \sum_{x,\mu\nu} \{1 - U_{\mu\nu}(x)\} + (\bar{\psi}_f, D_f[U^{6q_f} V]\psi_f)$$

$$U_\mu(x) = 1 + \frac{i}{6} A_\mu(x) + O(A^2)$$

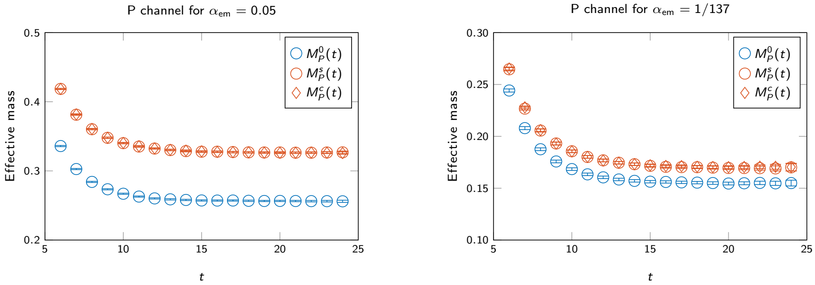
- Diracs interpolating operators can then be implemented as analytical functions of the link variables, e.g.

$$\Psi_f(x) = \frac{1}{3} \sum_{k=1}^{3} \psi_f(x) \prod_{s=0}^{L-1} U_k(x + sa\hat{k})^{-3q_f}$$

- The mass of, say, the charged kaon can be extracted from the fully gauge invariant correlator

$$\sum_{\mathbf{x}} \langle \bar{S}\gamma_5 U(t,\mathbf{x})\, \bar{U}\gamma_5 S(0)\rangle \simeq A(L) e^{-M_{K^+}(L) t}$$

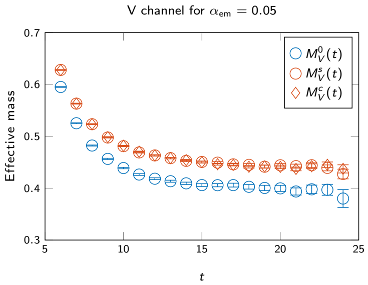
Some explorations

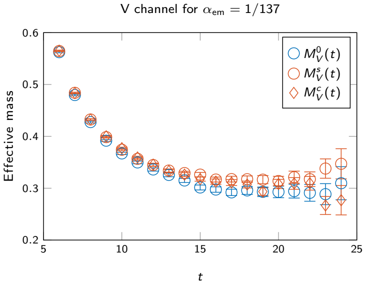


Full QCD+QED simulations (QCD parameters from CLS, Bruno, Korzec, Schaefer Phys. Rev. D 95 (2017))

$24^3 \times 48$	$\beta = 3.55$	$\kappa_f = \{0.137, 0.137, 0.137\}$
$a(\alpha_{em} = 0) = 0.0643(7)\text{fm}$	$L(\alpha_{em} = 0) = 1.54\text{fm}$	$M_{\pi,K}(\alpha_{em} = 0) = 420\text{MeV}$
$\alpha_{em} = \{0.05, 1/137\}$	$q_f = \{+2/3, 1/3, 1/3\}$	

Some explorations





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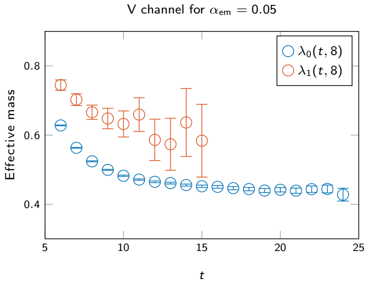
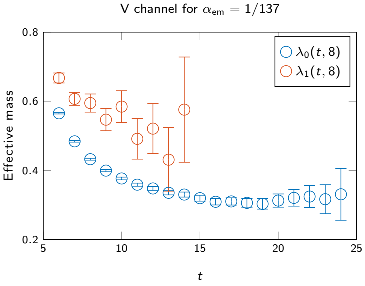
Real photons





$$V_k(t) = \frac{1}{2L^3} \sum_{\mathbf{x}} \{\bar{S}\gamma_k U(t, \mathbf{x}) - \bar{U}\gamma_k S(t, \mathbf{x})\}$$

$$W_k^l(t) = \sum_{\mathbf{p} \in O_h \bar{\mathbf{p}}} \tilde{P}(t, -\mathbf{p}) \epsilon_{k\ell j} p_\ell \tilde{A}_j^c(t, \mathbf{p})$$

$$\tilde{P}(t, \mathbf{p}) = \frac{1}{2L^3} \sum_{\mathbf{x}} e^{i\mathbf{p}\mathbf{x}} \{\bar{S}\gamma_5 U(t, \mathbf{x}) - \bar{U}\gamma_5 S(t, \mathbf{x})\}$$

$$\bar{\mathbf{p}} = \frac{\pi}{L}(1, 1, 1)$$

$$\tilde{A}_k^c(t, \mathbf{p}) = \frac{1}{L^3} \sum_{\mathbf{x}} e^{i\mathbf{p}\mathbf{x}} \triangle^{-1} \bar{\nabla}_j F_{jk}(t, \mathbf{x})$$

Crash intro to decay rates

Mostly nice pictures

Bloch-Nordsieck prescription

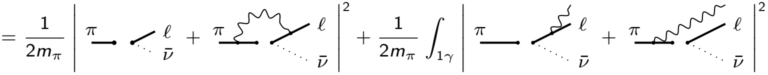
From the experimental point of view it is impossible to differentiate between

$$h \to \ell + \bar{\nu} \ ,$$
$$h \to \ell + \bar{\nu} + N\gamma \ ,$$

- if each photon is emitted with a lower energy than the detector resolution ΔE;
- and the total energy carryed away by the undetected photons is (roughly) less than the resolution ΔE with which we can reconstruct the lepton energy.

The physical quantity is the decay rate integrated over soft photons, which is finite.[1]

$$\Gamma(\Delta E) = \lim_{m_\gamma \to 0} \frac{1}{2m_\pi} \sum_{N=0}^{\infty} \frac{1}{N!} \int_{\substack{k_\alpha < \Delta E \\ \sum_\alpha k_\alpha < \Delta E}} \mathrm{d}\Phi_{N\gamma} \ |\langle \pi | \mathcal{H}_\mathrm{W} | \ell, \bar{\nu}, N\gamma \rangle|^2 =$$



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[1] The diagrammatic expansion is wrong. I am deliberately neglecting the wave-function renormalization for sake of presentation.

Bloch-Nordsieck prescription

From the experimental point of view it is impossible to differentiate between

$$h \to \ell + \bar{\nu} \ ,$$
$$h \to \ell + \bar{\nu} + N\gamma \ ,$$

Some kinematics:

$$P_h = P_\ell + P_\nu + \sum_{a=1}^{N} K_a \qquad P_h = (m_h, \mathbf{0}) \qquad P_\nu = \left[\frac{m_h^2 - m_\ell^2}{2m_h} - \epsilon\right](1, \mathbf{n}_\nu)$$

$$K_a = \frac{c_a m_h \epsilon}{E_\ell - \mathbf{p}_\ell \mathbf{n}_a}(1, \mathbf{n}_a) \qquad \sum_a c_a = 1 + O(\epsilon)$$

Effective Hamiltonian

$$\mathcal{H}_I(0) = \Psi^\dagger \nu(0)$$

Full system: QCD + photons + charged lepton + neutrinos

$$H = \tilde{H} + H_\nu \qquad \mathbf{P} = \tilde{\mathbf{P}} + \mathbf{P}_\nu$$

Decay rate

$$\Gamma\left(\frac{m_h^2 - m_\ell^2}{2m_h} - \epsilon < p_\nu < \frac{m_h^2 - m_\ell^2}{2m_h}\right) =$$

$$= \frac{\pi}{2m_h}\langle h|\Psi^\dagger(0)\frac{\delta(\tilde{H} + \tilde{P} - m_H)}{\tilde{P}}\chi_{[-\epsilon,0]}\left(\tilde{P} - \frac{m_h^2 - m_\ell^2}{2m_h}\right)\Psi(0)|h\rangle$$