Simon Eidelman School

Monte Carlo generators

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I hope to answer the following questions

- why do we need MC generators?
- what changes beyond LO?
- what effects dominate? can we do better?
- what is resummation?

If you have questions, now or later, get in touch! `yannick.ulrich@cern.ch`

why do we need MC generators?

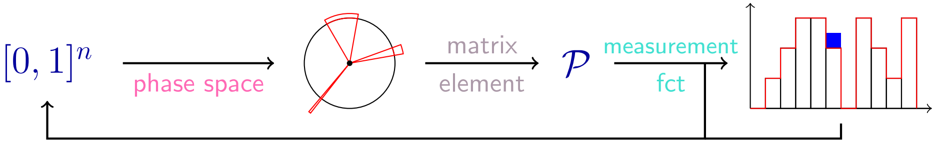
precision measurements

- we want to measure $a_\mu^{\rm HVP} \sim \int_{4m_\pi^2}^\infty \mathrm{d}s\ K(s) \times \sigma(ee \to \text{hadr})$
- precise measurements $\Rightarrow$ precise modelling for acceptance, fits, etc.
- analytic: possible but tedious & difficult

$\Rightarrow$ numeric solution using Monte Carlo to sample / integrate over phase space

- to first approximation eg. for $ee \to \mu\mu$: $\sigma = \int \mathrm{d}\Phi_{2\to 2}\ |\mathcal{A}^{(0)}_{2\to 2}|^2 \times S(\{p_i\})$

$$\sigma = \int \mathrm{d}\Phi_{2\to2}\, |\mathcal{A}^{(0)}_{2\to2}|^2 \times S(\{p_i\})$$



- the measurement function: experimental cuts, rejecting or accepting events as needed $\to$ will come back to this

... is knowing σ enough though?

- for simulations we need actually generate events according to $\mathrm{d}\mathcal{P} \sim \mathrm{d}\Phi_{2\to2}\, |\mathcal{A}^{(0)}_{2\to2}|^2$

sampling from a p.d.f. $\mathcal{P}(\{p_i\})$ is generally difficult... $\Rightarrow$ hit-and-miss sampling

- generate a random event $\{p_i\}$ and calculate $\mathcal{P}(\{p_i\})$
- generate a random number $r \in [0,1]$
- accept event if $r < \mathcal{P}(\{p_i\})/\max\mathcal{P}$

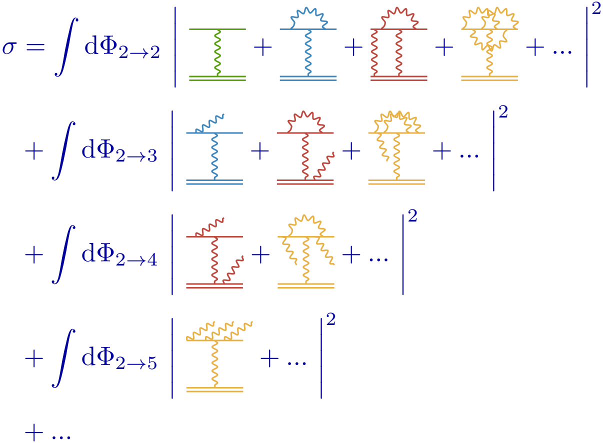
this can be quite wasteful

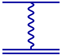
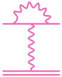
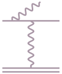
- need to find $\max\mathcal{P}$ by 'training' Monte Carlo
- if average weight $\langle\mathcal{P}\rangle \ll \max\mathcal{P}$, most events will be rejected
- various ways of optimising this: vegas [Lepage 80], foam [Jadach 02] normalising flow (eg. [Gao, Isaacson, Krause 20]), ...

- LO is not very precise

⇒ just expand higher in perturbation theory

- this is what's called fixed-order
- best ever ($gg \to H$ [Anastasiou, Duhr, Dulat, Herzog, Mistlberger 15]): NNNLO
- here: NNLO ($2 \to 2$) or NLO ($2 \to 3$) [Carloni Calame et al. 20; Banerjee, Engel, Signer, YU 20; Broggio et al 22]



$\sigma = \int \mathrm{d}\Phi_{2\to 2}\,\Big|$  $+$  $\Big|^2 \times S(\{p_i\}) + \int \mathrm{d}\Phi_{2\to 3}\,\Big|$  $\Big|^2 \times S(\{p_i, k\})$

- virtual matrix element: momentum flowing through the loop unconstrained
  $\Rightarrow$ integrate over it
- three-particle phase space: emitted photon can be hard or soft (high or low energy)
  $\Rightarrow$ even below the detector resolution!
- real matrix element: $\sim \dfrac{1}{(p_e \cdot k)} \sim \dfrac{1}{E_\gamma} \dfrac{1}{(1 - \beta_e \cos\theta_{e\gamma})}$
- real and virtual are separately divergent but their sum is finite (KLN theorem)

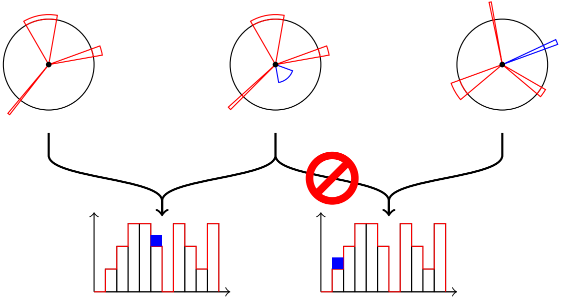
IR safety is not straightforward...

- measurement fct.: $S = 1$ to accept event, $S = 0$ rejects
- use this for histogramming $S \to S_1, ..., S_n$ for n bins
- event may have more particles (such as photons)
- what if the event has a soft photon?

$\Rightarrow$ cuts must not change for $k \to 0$ (soft safety)

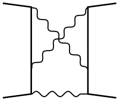
$\Rightarrow$ bin must also not change for $k \to 0$ (local soft safety)

- what about a collinear photon? (collinear safety)



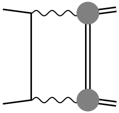
for leptons

- almost always done (semi)analytically
- can use decades of LHC tech, regulate by shifting $d \to 4 - 2\epsilon$
- fully automatised at one-loop (eg. [Buccioni et al. 19]), very difficult at two-loop
- bottleneck: calculation of so-called $\mathcal{O}(100)$ master integrals $\vec{I}(s_{ij})$
- currently favoured method: solve $\frac{\partial \vec{I}}{\partial s_{ij}} = M\vec{I}$, analytically or numerically (recent game changer: AMFlow [Liu, Ma, Wang 17])

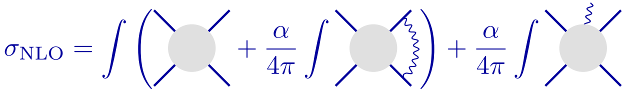


for hadrons

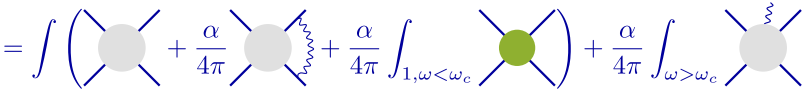
- the counting is a bit muddled, unclear what NNLO would mean
- different approaches: sQED, F×sQED, FsQED, GVMD, (maybe) full hadronic model in the future



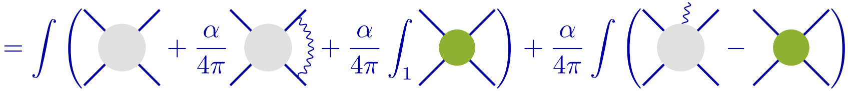
goal: regulate divergence & integrate real corrections numerically



- slicing: approximate radiation below cut-off

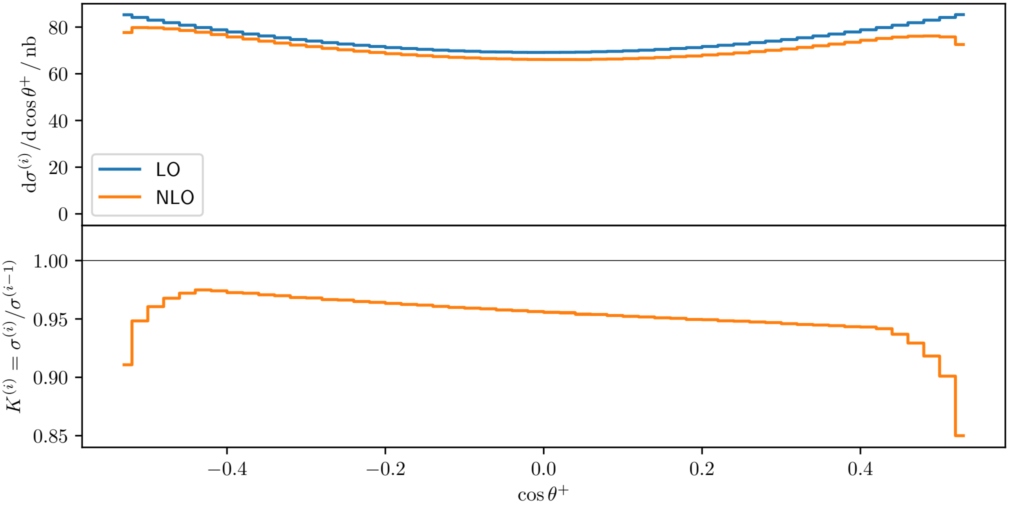


- subtraction: counter term to share singular structure

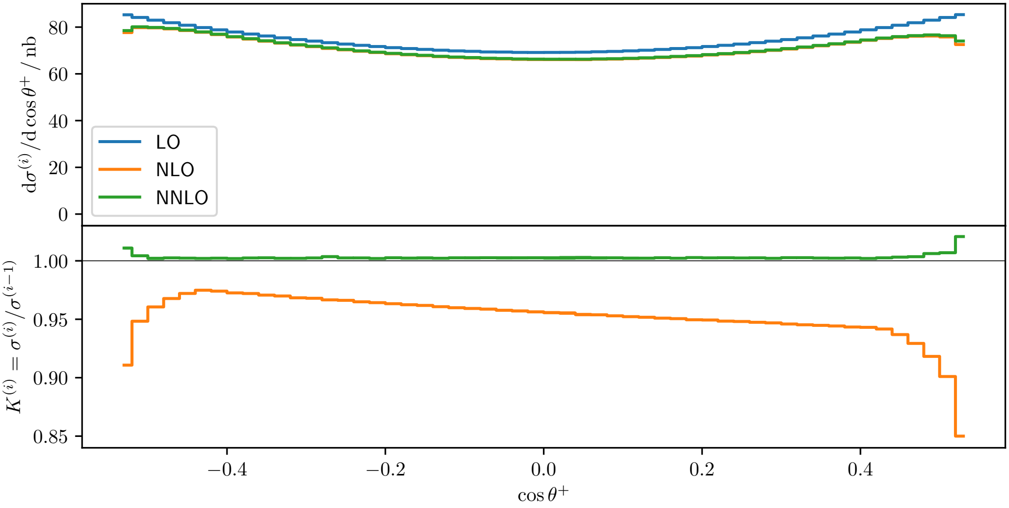


this works but generation now becomes very tricky!

$ee \to \mu\mu$ CMD-ish ($\sqrt{s} = 700\,\mathrm{MeV}$)



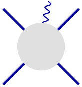
$ee \to \mu\mu$ CMD-ish ($\sqrt{s} = 700\,\mathrm{MeV}$)



MCMULE

why are these corrections so large?

$\alpha = 1/137$ so why do we see 10% corrections?

$$\sigma \sim \int$$  $$\sim \int \mathrm{d}\Phi_{2\to3}\,\frac{1}{E_\gamma^2}\,\frac{1}{1-\beta_e\cos\theta_{e\gamma}} \times S(\{p_i\})$$

- becomes large for $E_\gamma \to 0$ (even after slicing/subtraction) $\Rightarrow$ soft enhancement
- becomes large for $\theta_{e\gamma} \to 0$ because $\beta_e \sim 1 - 2m_e^2/s \Rightarrow$ collinear enhancement

$$\sigma \sim \frac{\alpha}{4\pi}\log\frac{1+\beta}{1-\beta}\;\log\frac{\omega_S^2}{s} \sim \frac{\alpha}{4\pi}\underbrace{\log\frac{m^2}{s}}_{L_m}\;\underbrace{\log\frac{\omega_S^2}{s}}_{L_s}$$

- ω_S depends on the measurement function $\Rightarrow$ L_s can be large but needn't be
- $L_m \sim 10$ almost always large

$\Rightarrow$ counting parameter is not $\alpha \sim 0.01$, it's $\alpha L \sim 0.1$!

don't expand in α, expand in αL!

- best ever (EEC in $ee \to$ jets, analytic, [Duhr, Mistlberger, Vita 22]): N^{4}LL
- numerically: NLL (eg. ALARIC [Herren et al. 23] & PanScales [van Beekveld et al. 22]), mostly LL(+) though
- our goal

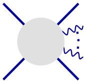
$$\sigma = \sum_{n_\gamma=0}^{\infty} \int \mathrm{d}\Phi_{2\to 2+n_\gamma} \Big| \sum_{\ell=0}^{\infty} \mathcal{A}^{(\ell)}_{2\to 2+n_\gamma} \Big|^2$$

- estimate $\mathcal{A}_{2\to 2+n_\gamma} \approx X_{n_\gamma} \times \mathcal{A}_{2\to 2}$ in some limit

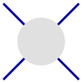
$$\begin{aligned}
\sigma =\ & \sigma_{0,0} && \text{LO}\\
& + \left(\frac{\alpha}{\pi}\right)^1 L^1 \sigma_{1,1} + \left(\frac{\alpha}{\pi}\right)^1 L^0 \sigma_{1,0} && \text{NLO}\\
& + \left(\frac{\alpha}{\pi}\right)^2 L^2 \sigma_{2,2} + \left(\frac{\alpha}{\pi}\right)^2 L^1 \sigma_{2,1} + \left(\frac{\alpha}{\pi}\right)^2 L^0 \sigma_{2,0} && \text{NNLO}\\
& + \left(\frac{\alpha}{\pi}\right)^3 L^3 \sigma_{3,3} + \left(\frac{\alpha}{\pi}\right)^3 L^2 \sigma_{3,2} + \left(\frac{\alpha}{\pi}\right)^3 L^1 \sigma_{3,1} + \left(\frac{\alpha}{\pi}\right)^3 L^0 \sigma_{3,0} && \text{NNNLO}\\
& \cdots && \text{N}^n\text{LO}
\end{aligned}$$

LL NLL NNLL $\cdots$ N^{n}LL

- soft limit for any number of loops & photons $\to$ eikonal $\mathcal{E}$ [Yennie, Frautschi, Suura 61]



$$\to \left(\prod_{i=1}^{n_\gamma} \underbrace{\frac{p_j \cdot p_k}{(p_j \cdot k_i)(p_k \cdot k)}}_{\mathcal{E}(k_i)} + \mathcal{O}(k_i^{-1}) \right) \times$$



- integration factorises, define $\hat{\mathcal{E}} = \int \mathrm{d}\Phi_\gamma \mathcal{E}$
- similarly for virtual, define $\check{\mathcal{E}} = \int \frac{1}{k^2} \frac{(2p_j - k)\cdot(2p_k + k)}{(k^2 - 2k\cdot p_k)(k^2 + 2k\cdot p_k)}$
- YFS form factor $Y = \hat{\mathcal{E}} + \check{\mathcal{E}}$ is finite

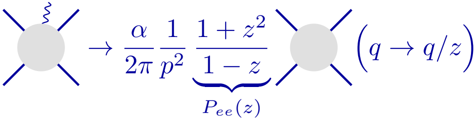
approximate all photons eikonal

$$\sigma = \sum_{n_\gamma=0}^{\infty} \int \mathrm{d}\Phi_{2\to 2+n_\gamma} \underbrace{\frac{1}{n_\gamma!} e^{-(-Y)}}_{\text{Poisson}} \Bigg(\prod_{i=1}^{n_\gamma} \mathcal{E}(k_i) \Bigg) |\mathcal{A}^{(0)}_{2\to 2}|^2$$

procedure:

- generate undressed event
- sample from Poisson distribution with $\langle n_\gamma \rangle \approx -Y$
- generate i-th photons according to $\mathcal{E}(k_i)$
- regenerate rest of event
- fix mistakes

- consider an off-shell electron $p^2 \neq m^2$ with energy E
- splitting function $P \equiv P_{ee}(z)$: probability of emitting a collinear photon s.t. energy is now $E_1 = zE$



- probability of radiating photon $E > z_{\text{min}} \times E$: $R(p^2) = \frac{\alpha}{2\pi}\frac{1}{p^2}\int_0^{1-z_{\text{min}}} \mathrm{d}z\ P_{ee}(z)$
- Sudakov factor $\Delta(s_1, s_2)$: probability of no resolvable radiation between $p^2 = s_1$ and $p^2 = s_2$

$$\Delta(s_1, s_2 + \delta s) = \Delta(s_1, s_2) \times \left(1 - \int_{s_2}^{s_2+\delta s} \mathrm{d}s\ R(s)\right)$$

Markov process

- start with some virtuality, eg. $s_1 = st/u$ [Carloni Calame et al. 00]
- find next virtuality s_{i+1} from $\Delta(s_i, s_{i+1}) = r \in [0,1]$
- find momentum fraction z, distributed according to $\mathcal{P} = \frac{\alpha}{2\pi} P(z)$
- keep doing this until $s_n = m^2$

modelling angular distribution [Carloni Calame 01]

- this just generates collinear photons
- can be improved by samplings angles from $\mathcal{E}$

can we just combine all of this?

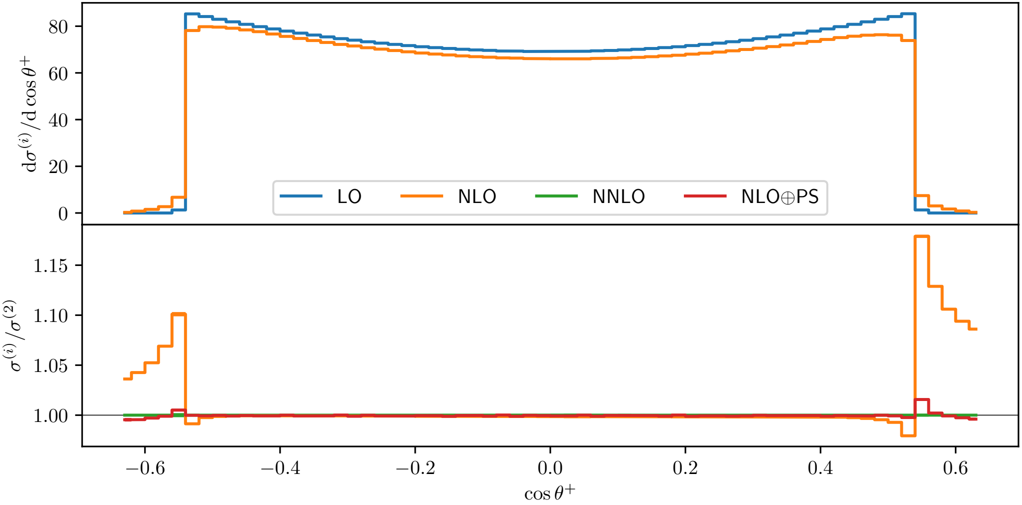
... sadly, not easily

- naively doing all of this (FO + YFS + PS) will result in double counting
- FO$\oplus$YFS is easy to any order in α, just use the actual matrix element rather than $\mathcal{E}$
- FO$\oplus$PS: understood at NLO [Balossini et al. 06], beyond WIP ("matching")
- "PS$\oplus$YFS": can use $\mathcal{E}$ for angles in PS or P_{ee} for matrix elements in YFS

beyond photons

- for finiteness, only photon radiation is required
- what about pair production $ee \to XX + ee, \mu\mu, \pi\pi, \tau\tau, ...$?
- can be physically separated as long as $m_f > 0$
- might be kinematically surpressed / impossible, depending on s
- but: corrections $\sim \log \frac{m_f^2}{s}$!
- combining with corresponding virtual actually reduces corrections for $f = e$
- possible to capture efficiently using eg.
  - PS with other splittings such as $P_{e\gamma}$ ($\gamma \to ee$)
  - YFS (can be viewed as YFS⊕PS) [Flower, Schönherr 22]

$ee \to \mu\mu$ CMD-ish ($\sqrt{s} = 700\,\mathrm{MeV}$) [FO: McMule, PS: BabaYaga@NLO]



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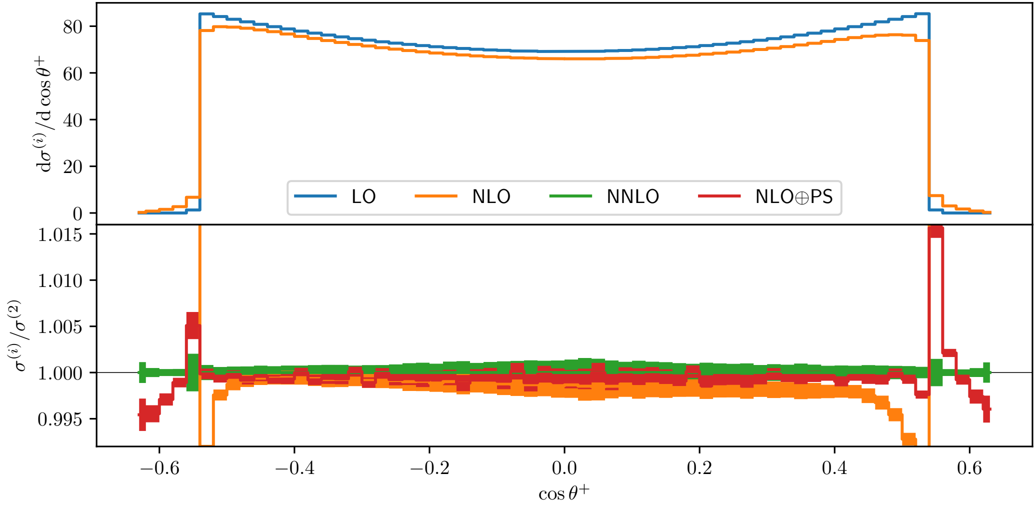


- in QCD: four-pt scale variation (full result does not depend on $\mu \to$ theory error $\approx$ scale dependence)
- doesn't really work for QED
- compare codes that do different things (assuming correctness & validity)
  - all PS have the same LL but different parts of the NLL
  - FO vs. truncated PS: missing higher order
  - PS vs. FO: dominant effects in PS
- all of this is really tricky & difficult...

$\Rightarrow$ most codes will not give you a theory error, just a statistical error (that may very well be underestimated!)

in the end, the only way to estimate missing effects is to calculate them and note their size

- MC are very important
- choice of tool non-trivial, depends on situation
- ideally compare multiple codes and see what matters for your experiment
- advertisements
  - I work on a FO-NNLO code called McMule, YFS WIP (LL, maybe even NLP)

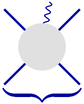
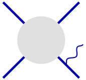
    `https://mule-tools.gitlab.io`
  - RadioMonteCarLow 2: effort to provide better codes to $ee \to$ stuff at $s \sim (\text{few GeV})^2$.

    `https://radiomontecarlow2.gitlab.io`

a non-exhaustive list of resource I've used for this

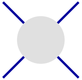
- RadioMonteCarlow 2 review (draft online now)
- structure functions (analytic resummation in QED) [Beenakker, Berends, van der Marck 90]
- initial state QED for e^+e^- review [Snowmass 22]
- broad generators for high-energy physicsi review [Snowmass 22]
- review of state-of-the-art for μ-e scattering [Banerjee et al. 20]
- Parton showers for QED [Carloni Calame 01]
- various diploma & PhD theses
- Books: QCD and Collider Physics & The Black Book of Quantum Chromodynamics
- Tasi lecture on parton shower event generators [Höche 14]

here: at tree-level, full proof in modern notation see eg. [Engel 22]

$\mathcal{A}^{(0)}_{n+1} =$  $+ \sum_{\text{leg}}$  $= \sum_i \Big(\Gamma_i(p_i - k) \frac{\not p_i - \not k + m}{(p_i-k)^2 - m_i^2} \gamma^\mu u(p_i) \Big) \epsilon^\mu + \mathcal{O}(k^0)$

$$\overset{*}{=} \sum_i \Big(\Gamma_i(p_i) \frac{\not p_i + m_i}{2 p_i \cdot k} \gamma^\mu u(p_i) \Big) \epsilon^\mu + \mathcal{O}(k^0)$$

$$\overset{\dagger}{=} \sum_i \Big(\Gamma(p) \frac{2p^\mu + \gamma^\mu(-\not p_i + m_i)}{2 p_i \cdot k} u(p_i) \Big) \epsilon^\mu + \mathcal{O}(k^0)$$

$\overset{\#}{=}$  $\times \sum_i \frac{p_i \cdot \epsilon}{p_i \cdot k} + \mathcal{O}(k^0)$

$*$ drop terms k^0, $\dagger$ anticommute $\{\not p_i, \gamma^\mu\} = 2p_i^\mu$, # Dirac equation $(\not p - m)u = 0$

when generating we've made the following mistakes, reweight as follows

- used the undressed q_j eikonals to generate photons instead of dressed p_j:
  $$W_{\text{dipole}} = \prod_i \frac{\mathcal{E}(\{p_j\}, k_j)}{\mathcal{E}(\{q_j\}, k_j)}$$
- used e^{-n_γ} instead of n^Y when generating n_γ: $W_{\text{YFS}} = \exp(Y + \langle n \rangle)$
- depending on how event is generated, other corrections might be needed as well (Lorentz boost, momentum mapping etc.)

angular distribution

- we need to sample θ and ϕ according to $\mathcal{E}$
- common strategy: pick one dipole of particles i and j and sample θ in dipole frame according to $\mathcal{E}_{ij} = \dfrac{p_i \cdot p_j}{p_i \cdot k \, p_j \cdot k}$

- probability of radiating: $R(p^2) = \frac{\alpha}{2\pi}\frac{1}{p^2}\int_0^{1-z_{\text{min}}} \mathrm{d}z\ P_{ee}(z)$
- probability of not radiating between s_1 and s_2: $\Delta(s_1,s_2)$ (per definition)
- going a small step further $s_2 \to s_2+\delta s$: probabilites multiply

$$\Delta(s_1,s_2+\delta s) = \underbrace{\Delta(s_1,s_2)}_{[s_1,s_2]} \times \underbrace{\left(1-\int_{s_2}^{s_2+\delta s}\mathrm{d}s\ R(s)\right)}_{[s_2,s_2+\delta s]} \approx \Delta(s_1,s_2) - \Delta(s_1,s_2)\ \delta s\ R(s_2)$$

- this is a differential equation $\frac{\mathrm{d}\Delta(s_1,s_2)}{\mathrm{d}s_2} = -R(s_2)\Delta(s_1,s_2)$
- solved by $\Delta(s_1,s_2) = \exp\left(-\int_{s_1}^{s_2}\frac{\mathrm{d}s}{s}\int_0^{1-z_{\text{min}}}\mathrm{d}z\frac{\alpha}{2\pi}P_{ee}(z)\right)$