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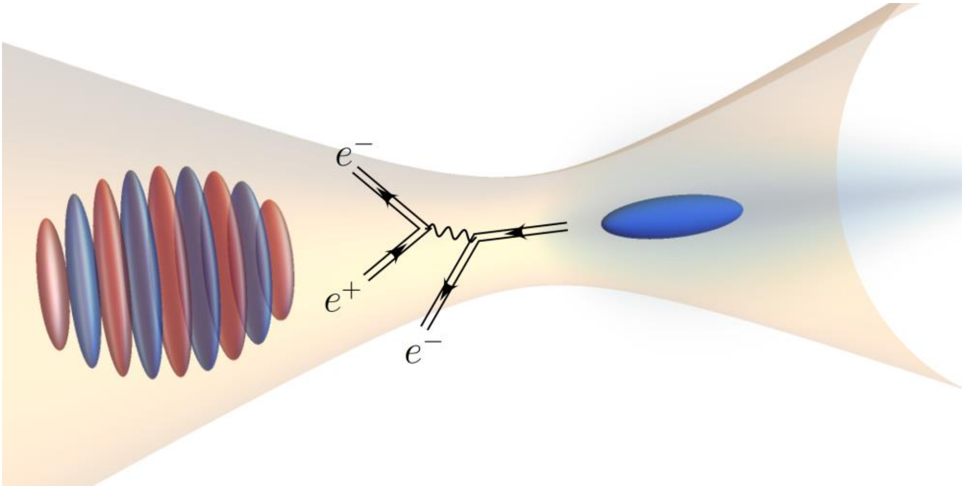
Simulations Q&A



Tom Blackburn
Department of Physics, University of Gothenburg
www.gu.se/en/research/plasma-physics

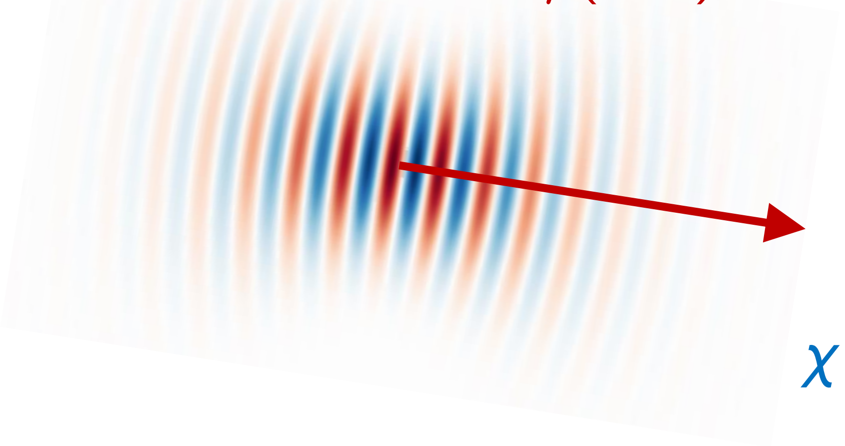
3 December 2024

SFQED Workshop, DESY

Problem statement

Laser defined by normalised amplitude

$a_0 = eE/(m\omega)$



High-energy electron (or photon)

Collision defined by:

(centre of mass) energy parameter

$\eta = \gamma(1 + \cos\theta)\omega/m,$

quantum nonlinearity parameter

$\chi = a_0\eta = \gamma(1 + \cos\theta)E/E_{\mathrm{Sch}}$

Problem statement

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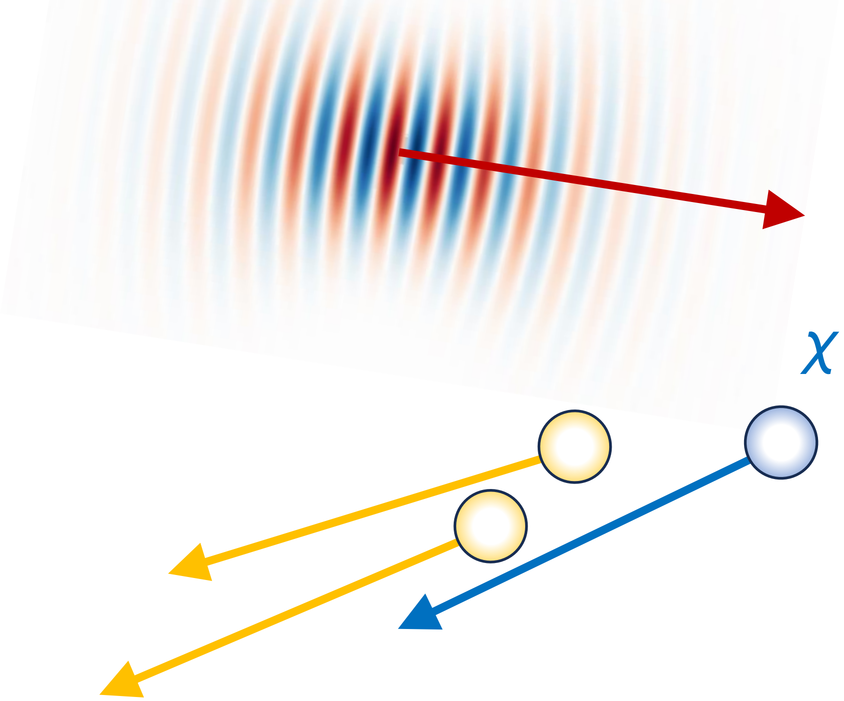

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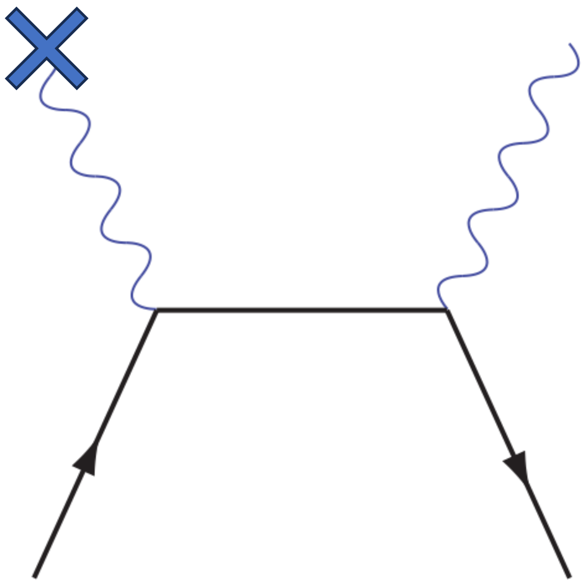
High-energy electron (or photon)

For $a_0 > 1$ (multiphoton) and $\chi > 1$ (quantum), determine the differential probabilities of all possible final states, going to arbitrarily high multiplicity.

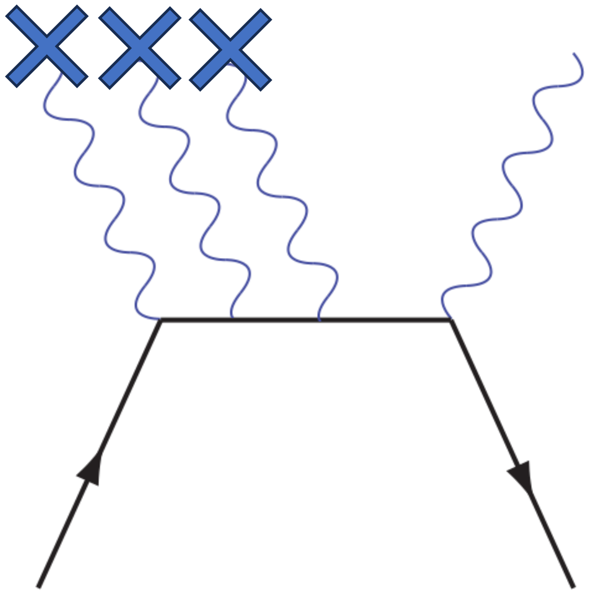
Interaction with the background field



At lowest order, draw one photon from the laser to emit one high-energy photon (a gamma ray): **linear** Compton scattering

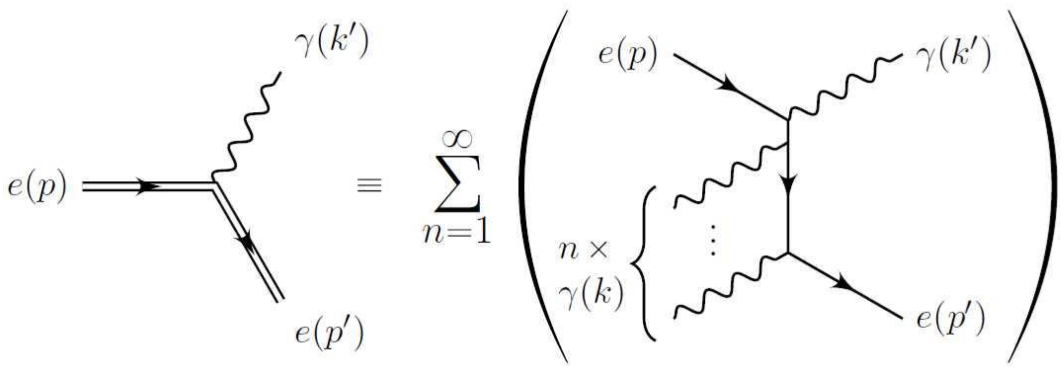
At the probability level, first vertex carries a factor

$\alpha I \sim (eE)^2 \sim {a_0}^2$



Nonlinear Compton scattering

Interaction with the background field



Probability if $\chi \ll 1$:

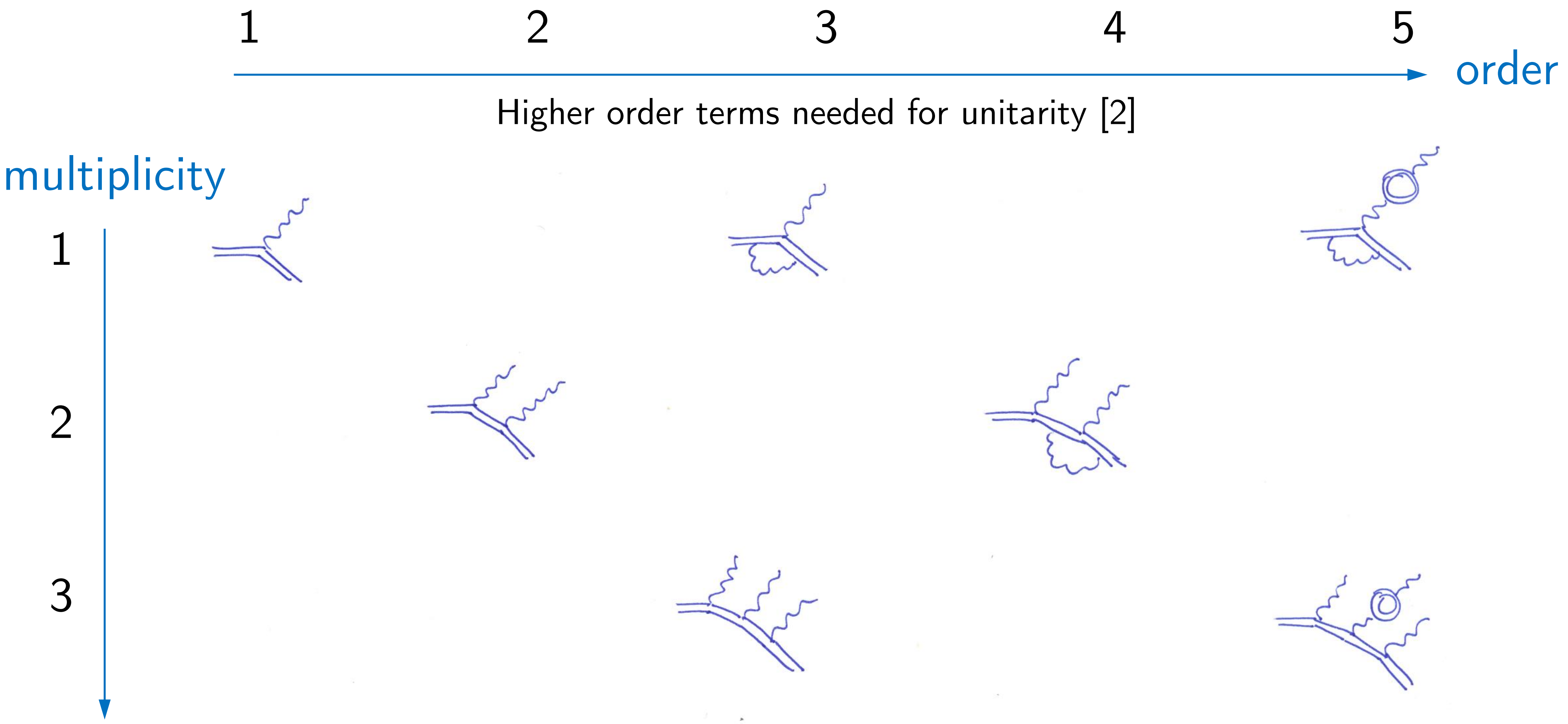
$$\alpha\chi\tau/\eta \sim \alpha a_0 \tau$$

Probability if $\chi \gg 1$:

$$\alpha\chi^{2/3}\tau/\eta$$

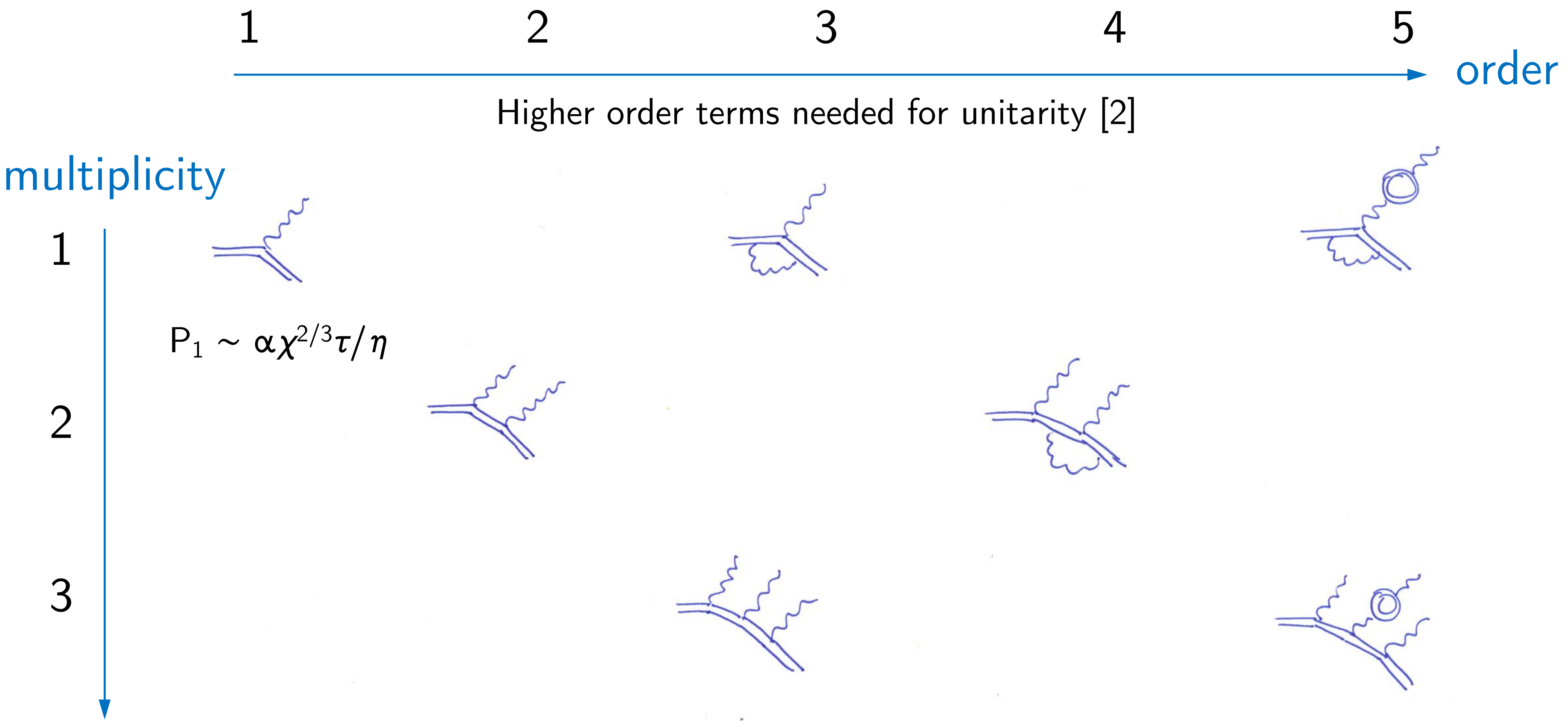
- Solve Dirac equation for the background field to obtain new basis states (plane EM wave = Volkov states).
- The probability current coincides with classical solution of the Lorentz force equation.
- Construct Feynman rules as usual and expand perturbatively in the coupling to the radiation field, α.

Interaction with the radiation field



[1] Morozov, Narozhny and Ritus, JETP 53, 1103 (1981)
[2] Ilderton and Torgrimsson, PLB 725, 481 (2013); Heinzl, Ilderton and King, PRL 127, 061601 (2021)

Interaction with the radiation field



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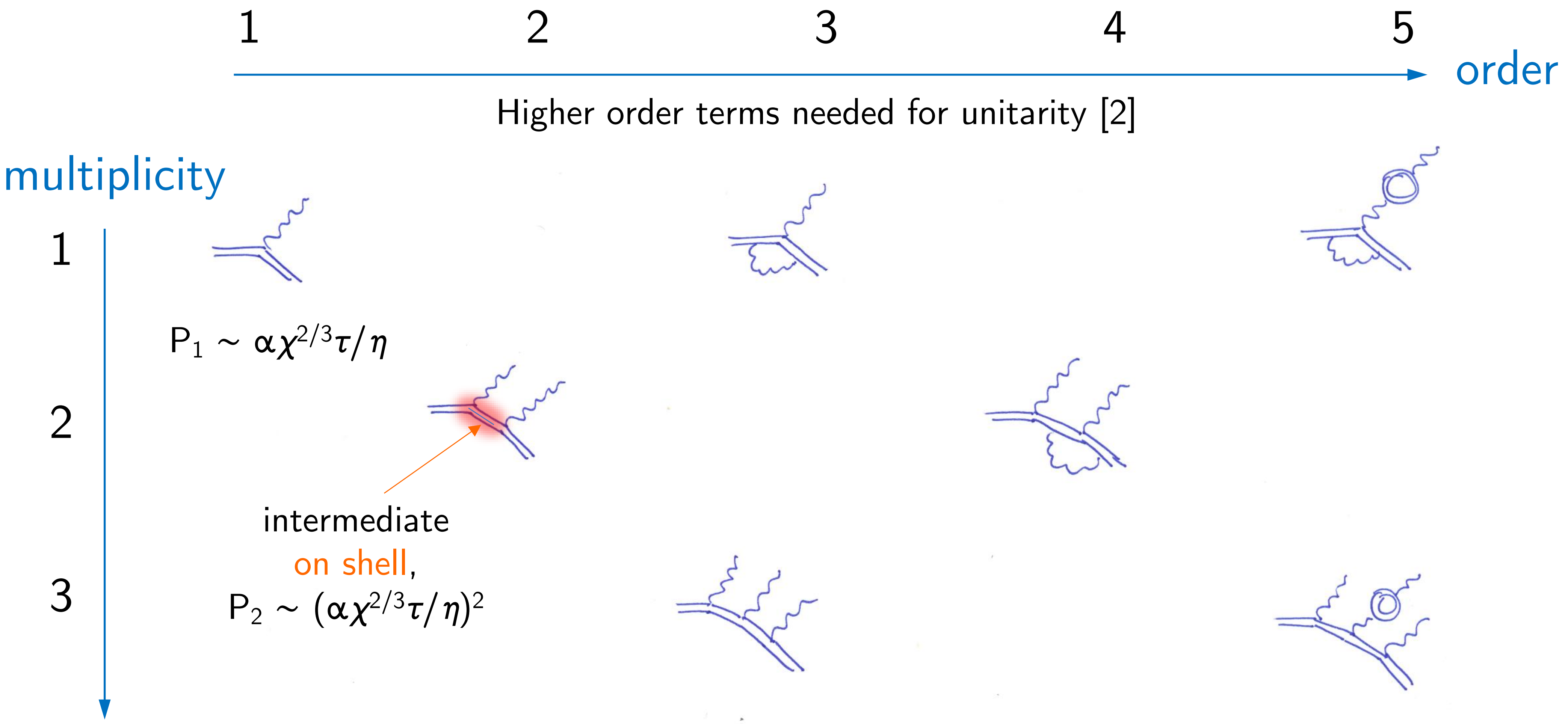

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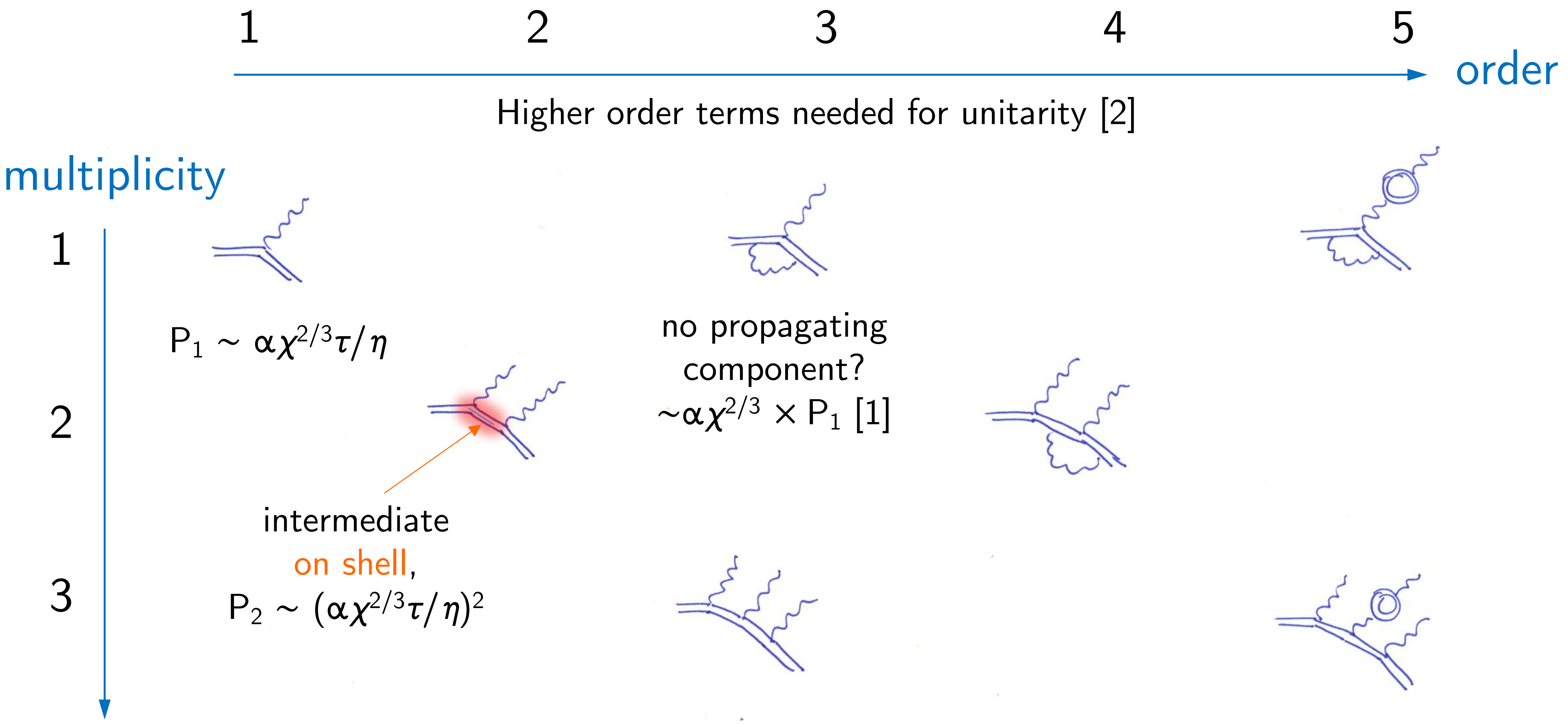

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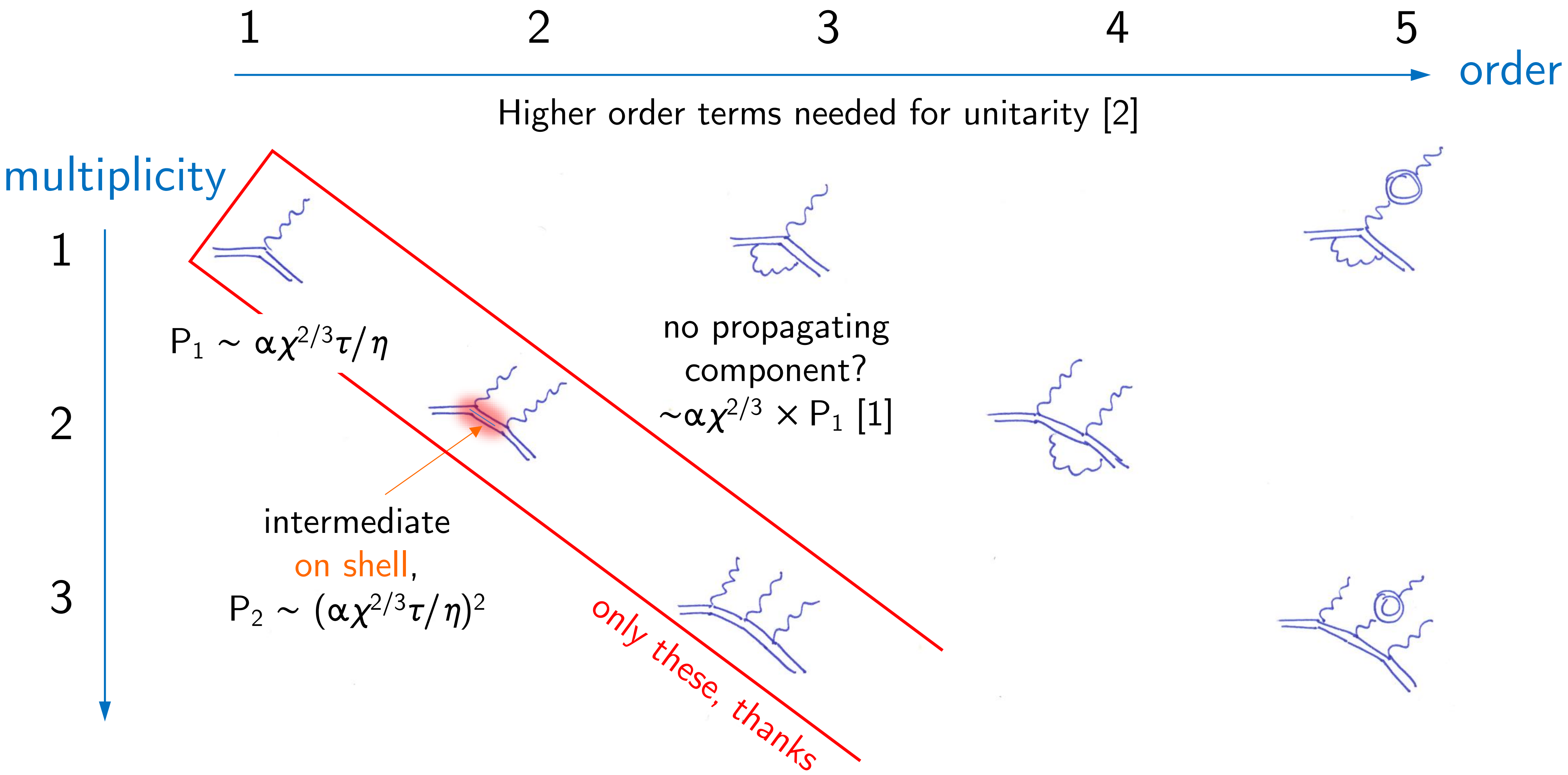
Interaction with the radiation field



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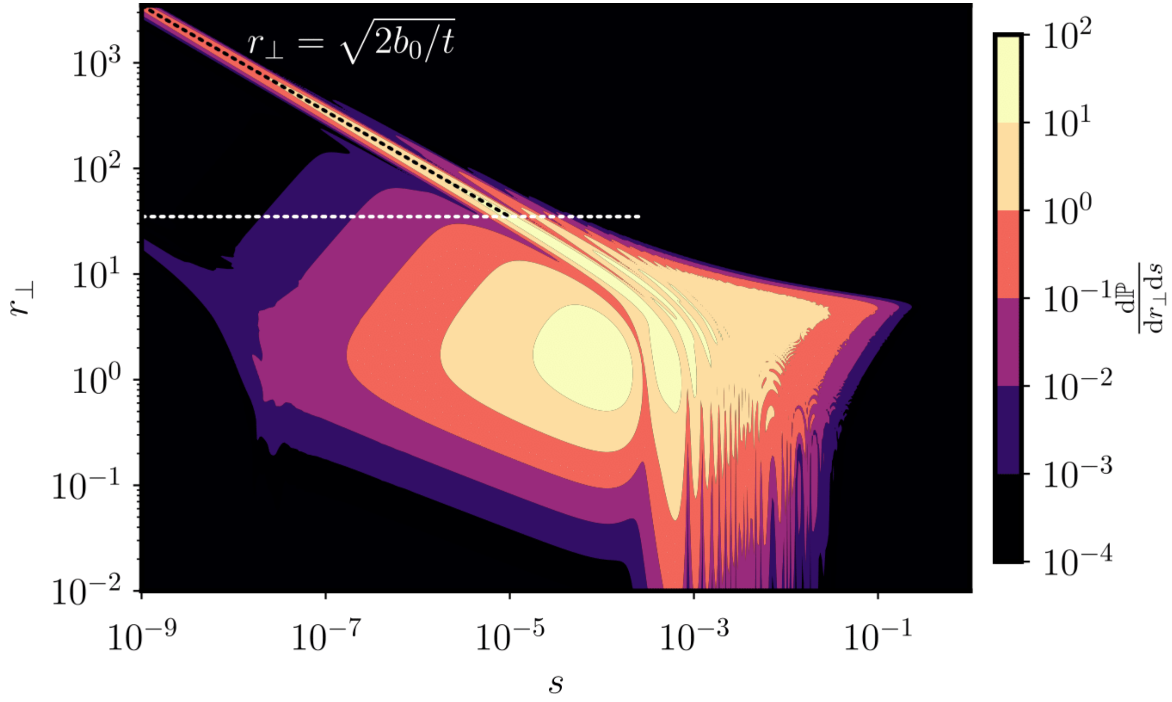
Simulations Q&A

What can theory tell us?

$$\frac{d^3\mathbb{P}}{df\, d^2\mathbf{r}_\perp} = \frac{\alpha m^2}{(4\pi\omega_0 p^+)^2}\frac{f}{1-f}\frac{1}{2}\sum_{\text{spin,pol}}\left|\sum_j \mathscr{T}_j\mathscr{C}_j\right|^2$$



Ilderton et al, PRA 99, 042121 (2019)

- Fundamental approach: treat interaction with laser field exactly (i.e. nonperturbatively) and expand perturbatively in the dynamical EM field (i.e. the high-energy photons).
- Limitations: transition between asymptotic states → complete knowledge of background field required, can't do arbitrary field configurations, backreaction neglected, multiplicity (# particles in final state).

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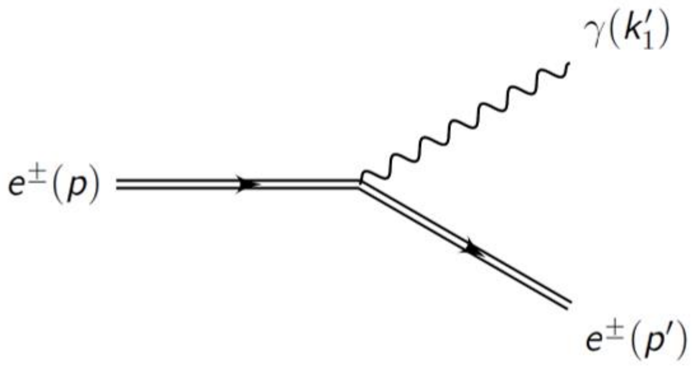
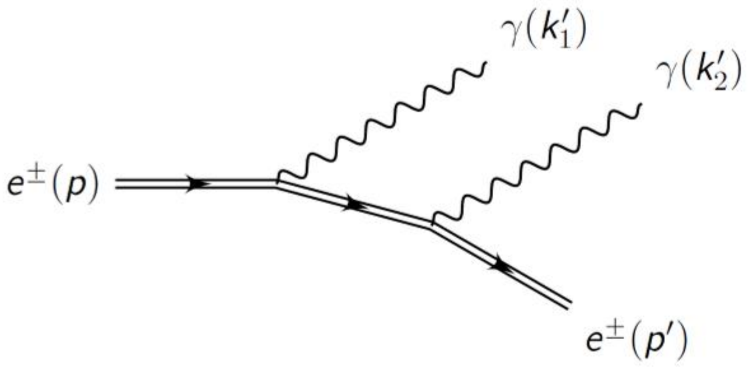
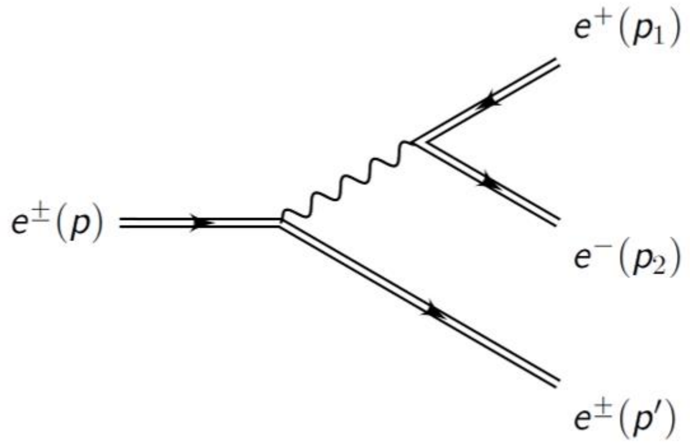
Simulations Q&A

What can theory tell us?

electron-seeded + pulsed plane wave:







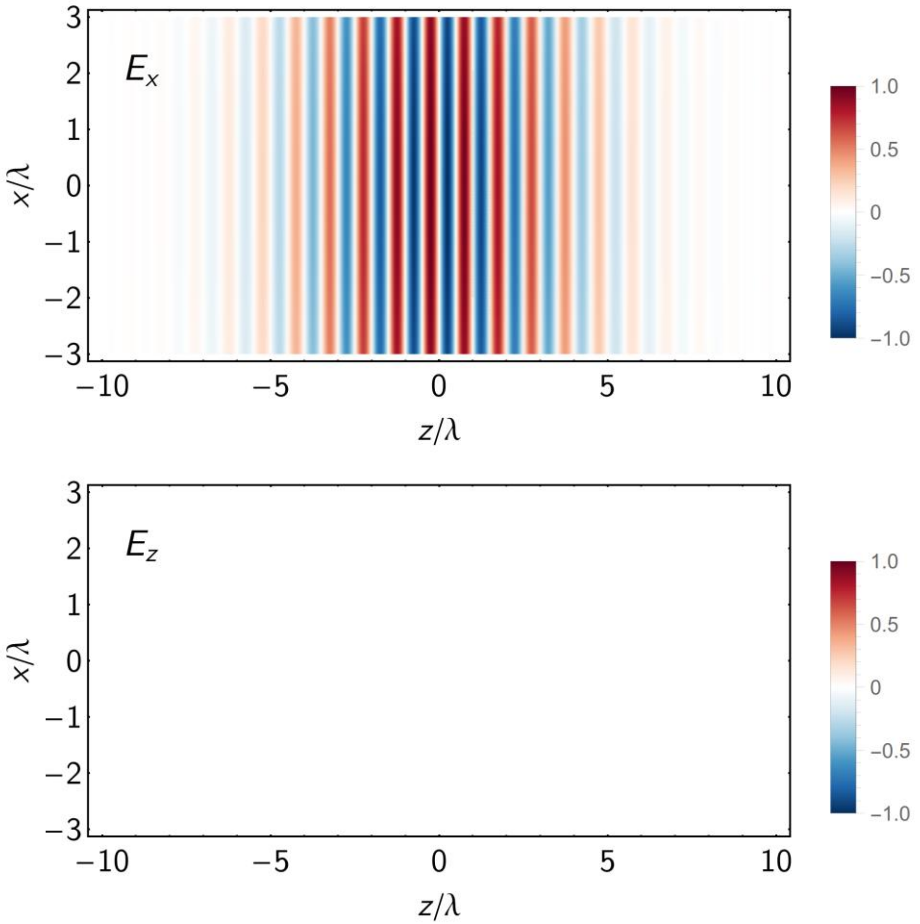
Narozhnyi and Fofanov, Sov Phys JETP 83, 14 (1996)
Boca and Florescu, PRA 80, 053403 (2009)
Harvey, Heinzl and Ilderton, PRA 79, 063407 (2009)
Mackenroth, Di Piazza and Keitel, PRL 105, 063903 (2010)
Heinzl, Ilderton and Marklund, PLB 692, 250 (2010)
Krajewska and Kaminski, PRA 85, 062102 (2012)
... and many more

Lötstedt and Jentschura, PRL 103, 110404 (2009)
Seipt and Kämpfer, PRD 85, 101701 (2012)
Mackenroth and Di Piazza, PRL 110, 070402 (2013)
King, PRA 91, 033415 (2015)
Dinu and Torgrimsson, PRD 99, 096018 (2019)

Hu, Muller and Keitel, PRL 105, 080401 (2010)
Ilderton, PRL 106, 020404 (2011)
King and Ruhl, PRD 88, 013005 (2013)
Dinu and Torgrimsson, PRD 97, 036021 (2018)
King and Fedotov, PRD 98, 16005 (2018)
Mackenroth and Di Piazza, PRD 98, 116002 (2018)
Dinu and Torgrimsson, PRD 102, 16018 (2020)

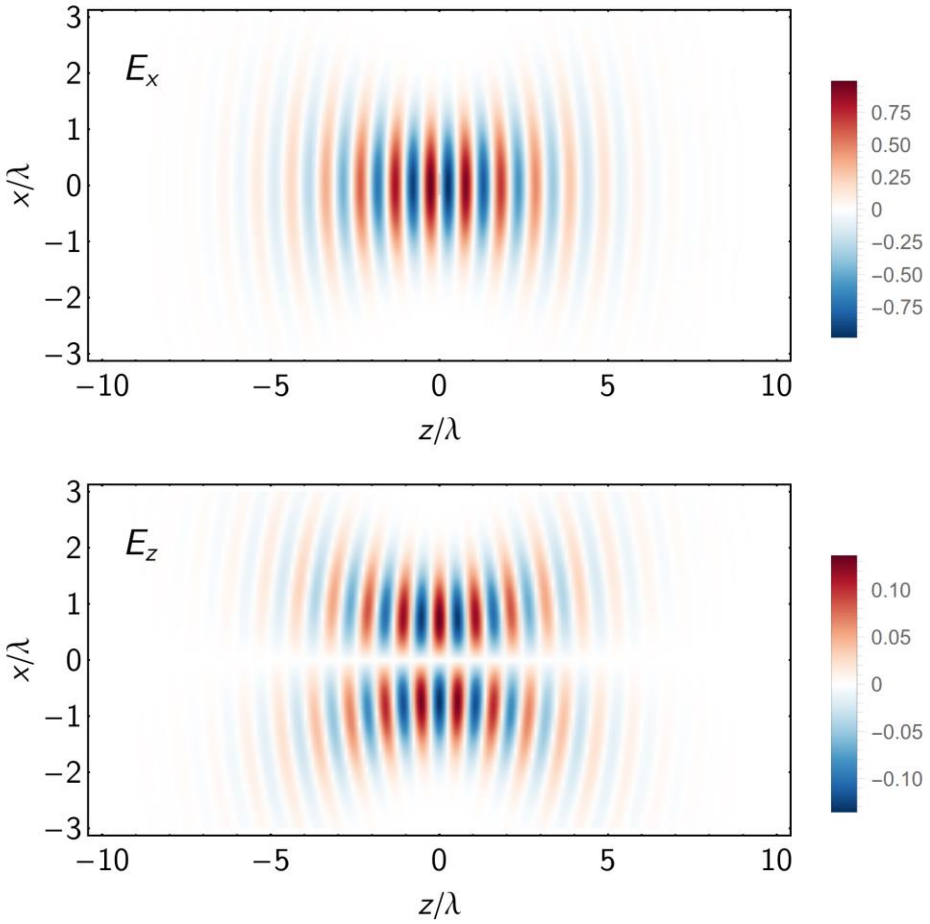
Also: resummation techniques for very high-order processes

Beyond plane waves



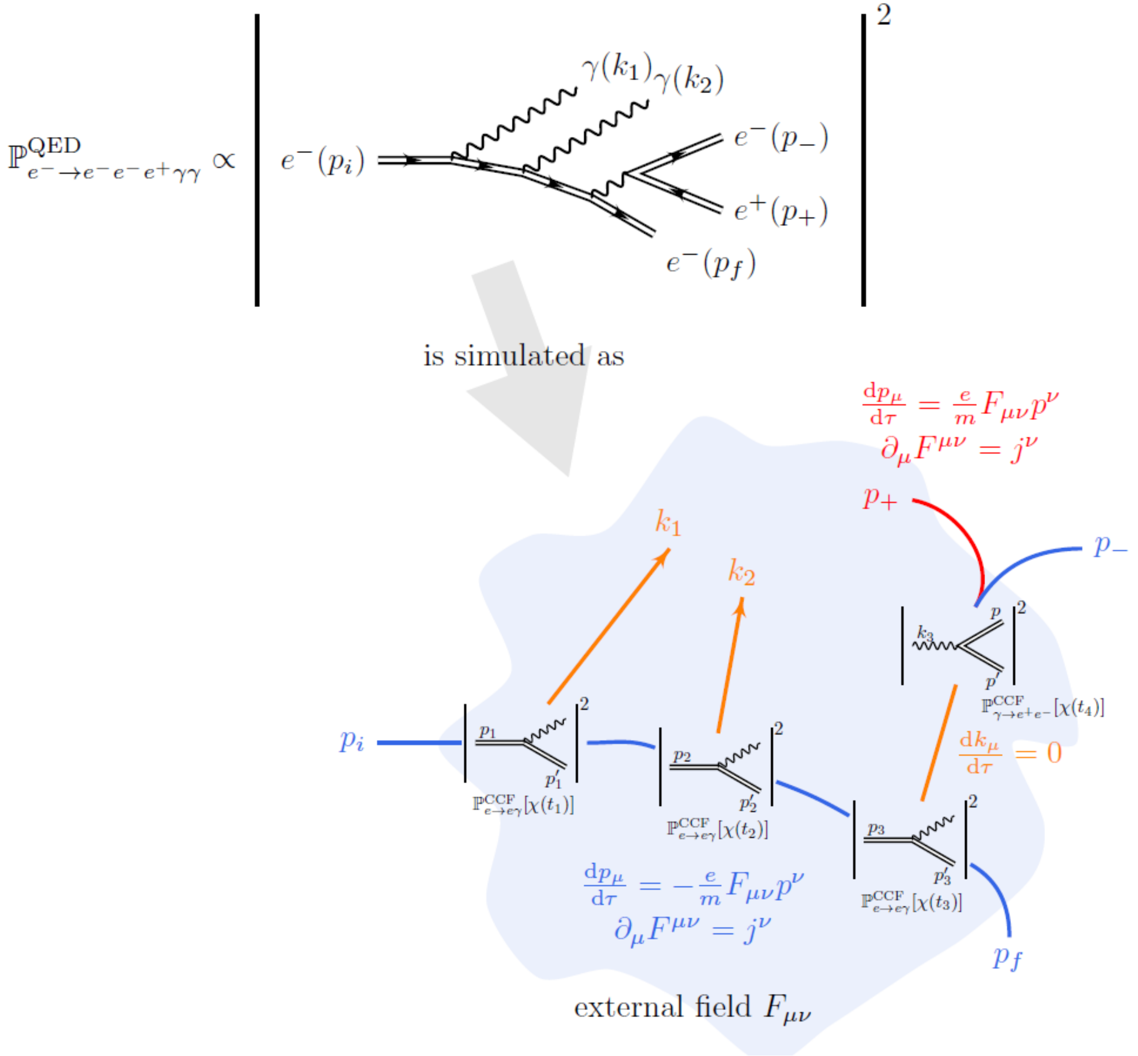
- The plane wave is the paradigmatic choice of background for calculations of nonlinear classical and quantum processes in strong electromagnetic fields.
- Classical and quantum dynamics of an electron in a plane-wave background are exactly solvable [see, for example, Heinzl and Ilderton, PRL 118, 113202 (2017)]

Beyond plane waves



- Lasers reach high intensity by focusing – getting close to the diffraction limit
- A focusing electromagnetic pulse has to be described numerically (usually with a certain degree of approximation).
- No complete theory for QED interactions exists in this background. High-energy approximations possible [Di Piazza, PRL 113, 040402 (2014)]

Local approximations



- QED rates in the LCFA / LMA + point-like emission events linked by classical trajectories that are determined by Lorentz force / ponderomotive force equation.
- Higher-order processes are broken down into a chain of first-order processes.
- Requires $a_0 \gg 1$ (strictly, $a_0^3/\chi \gg 1$) or sufficiently long pulses.

How do we study strong EM fields? (Theory)

Probability rates

$$\frac{dP}{dk_-} = -i\frac{\alpha}{2\pi}\frac{1}{p_-}\frac{\xi_0}{\chi_0}\int\frac{d\varphi d\varphi'}{\varphi-\varphi'+i0}\left\{1+\frac{p_-^2+p_-'^2}{4p_-p_-'}[\boldsymbol{\xi}_\perp(\varphi)-\boldsymbol{\xi}_\perp(\varphi')]^2\right\}$$
$$\times\exp\left\langle i\frac{1}{2}\frac{k_-}{p_-'}\frac{\xi_0}{\chi_0}\left\{\varphi-\varphi'+\int_{\varphi'}^{\varphi}d\tilde{\varphi}\,\boldsymbol{\xi}_\perp^2(\tilde{\varphi})-\frac{1}{\varphi-\varphi'}\left[\int_{\varphi'}^{\varphi}d\tilde{\varphi}\,\boldsymbol{\xi}_\perp(\tilde{\varphi})\right]^2\right\}\right\rangle$$

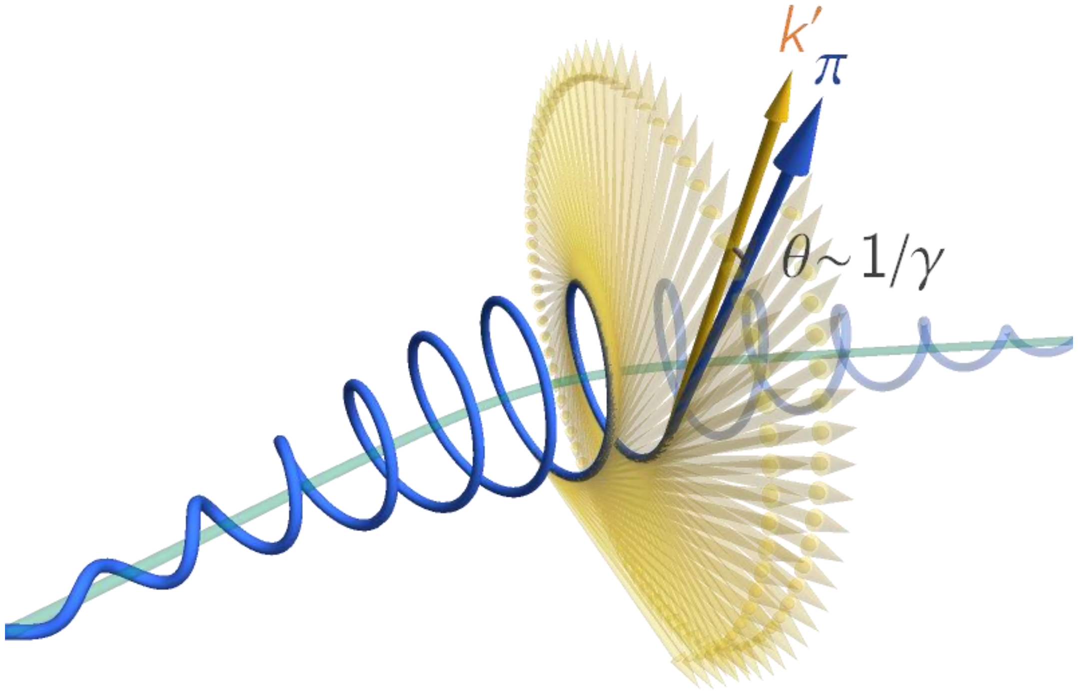
$$\frac{dP}{dk_-d\varphi_+} = \frac{\alpha}{2\pi}\frac{1}{p_-}\frac{\xi_0}{\chi_0}\mathrm{Im}\int\frac{d\varphi_-}{\varphi_-+i0}\left\{1+\frac{p_-^2+(p_--k_-)^2}{4p_-(p_--k_-)}\left[\boldsymbol{\xi}_\perp\left(\varphi_+-\frac{\varphi_-}{2}\right)-\boldsymbol{\xi}_\perp\left(\varphi_++\frac{\varphi_-}{2}\right)\right]^2\right\}e^{i\Phi(k_-,\varphi_-,\varphi_+)},$$

$$\Phi(k_-,\varphi_-,\varphi_+) = \frac{1}{2}\frac{k_-}{p_--k_-}\frac{\xi_0}{\chi_0}\left\{\varphi_-+\int_{-\varphi_-/2}^{\varphi_-/2}d\tilde{\varphi}\,\boldsymbol{\xi}_\perp^2(\varphi_++\tilde{\varphi})-\frac{1}{\varphi_-}\left[\int_{-\varphi_-/2}^{\varphi_-/2}d\tilde{\varphi}\,\boldsymbol{\xi}_\perp(\varphi_++\tilde{\varphi})\right]^2\right\},$$

from Di Piazza et al, PRA 98, 012134 (2018)

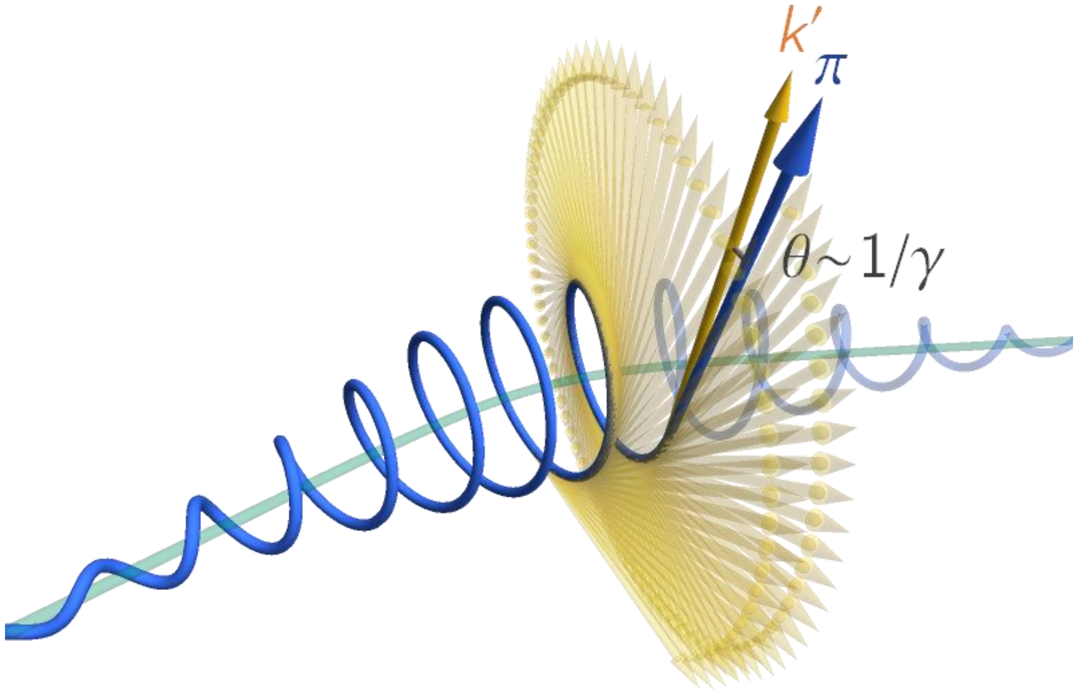
- Probability for a single-vertex process is given by a double integral over phase variables φ_1 and φ_2.
- Exchange for average phase $\varphi_{av} = (\varphi_1 + \varphi_2)/2$ and interference phase $\varphi = (\varphi_1 - \varphi_2)/2$.
- In the limit that the interference phase is small, the probability is a single integral over a probability rate.

Adding QED to classical simulations



- Conventional (whether single-particle or PIC) codes that model strong-field QED processes are "semiclassical."
- Particles have well-defined trajectories.
- QED events occur non-deterministically according to the relevant probability rate, along this trajectory.

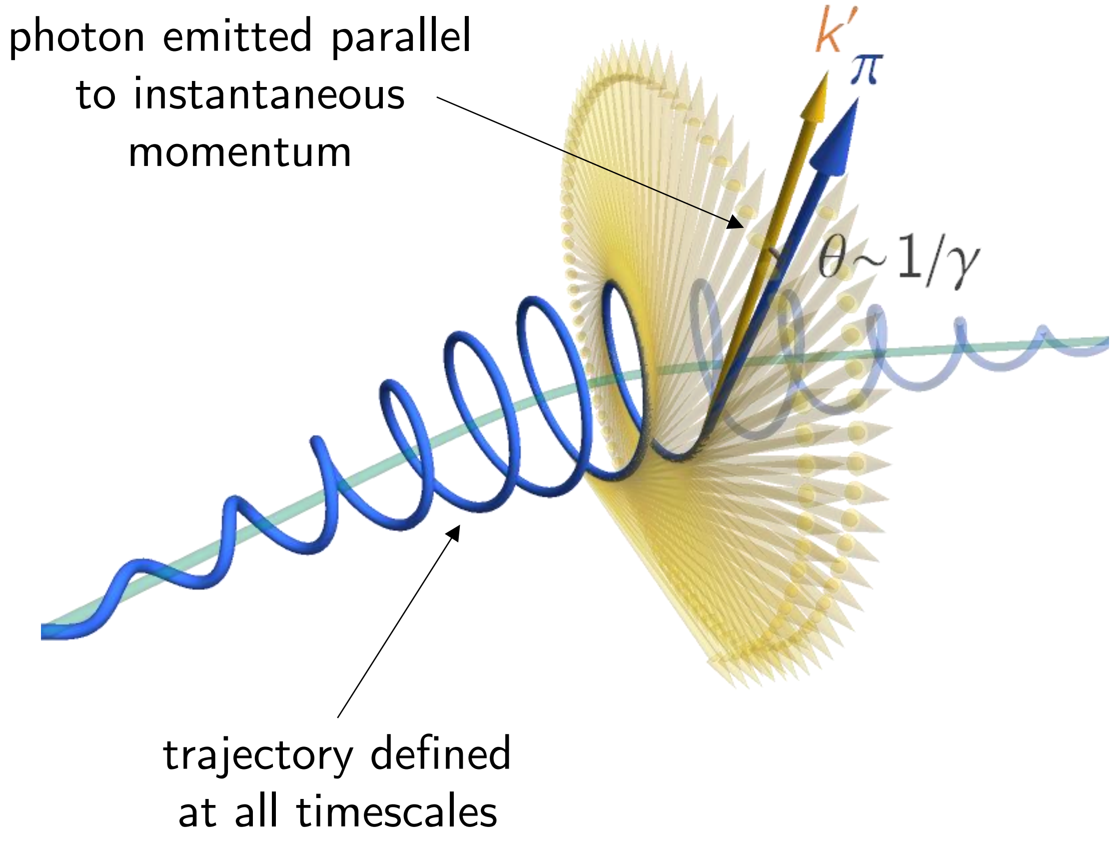
Using the LCFA



- The standard approach is based on the locally constant field approximation.
- Rate calculated for a constant, crossed background.
- Quantity that enters the rate is the instantaneous (kinetic) momentum π^μ and the quantum parameter χ.
- Equation of motion is the Lorentz force $\dot{\pi}^\mu = -\mathrm{e}\, F^{\mu\nu}\pi_\nu/m$.

What if a_0 is not large?

Using the LCFA



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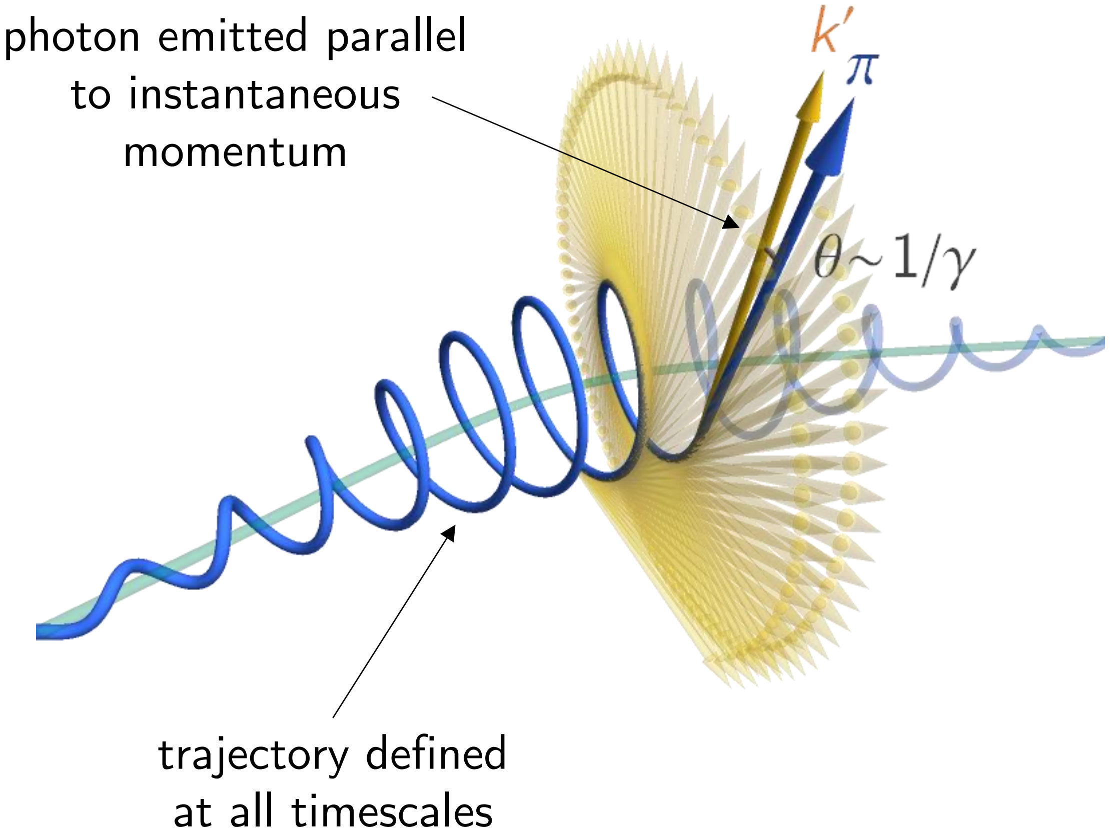
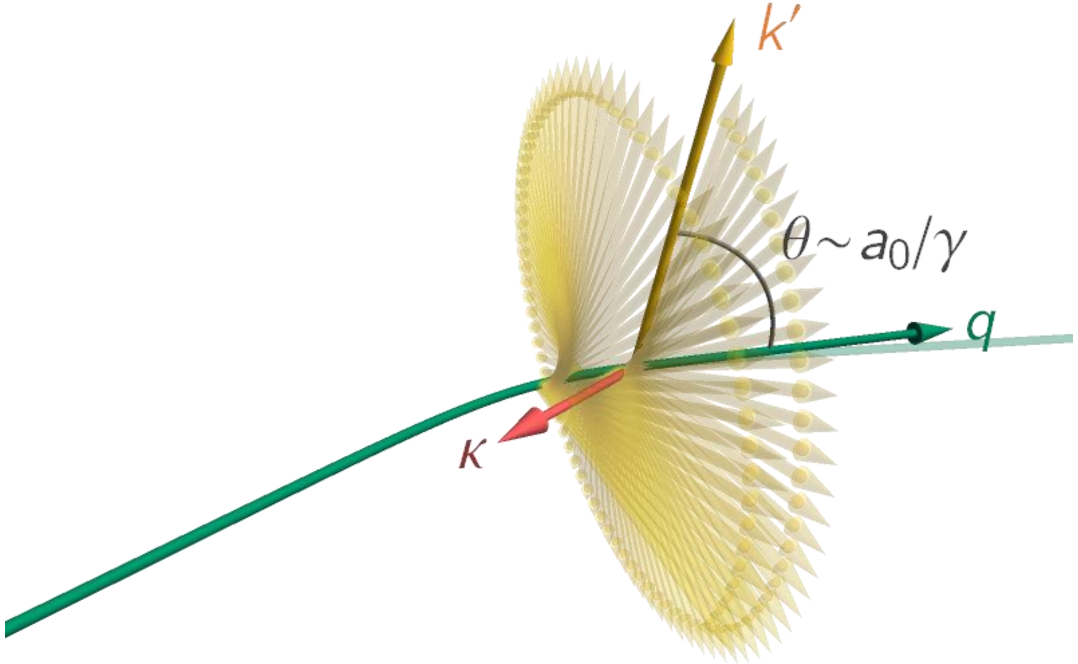
Using the LCFA



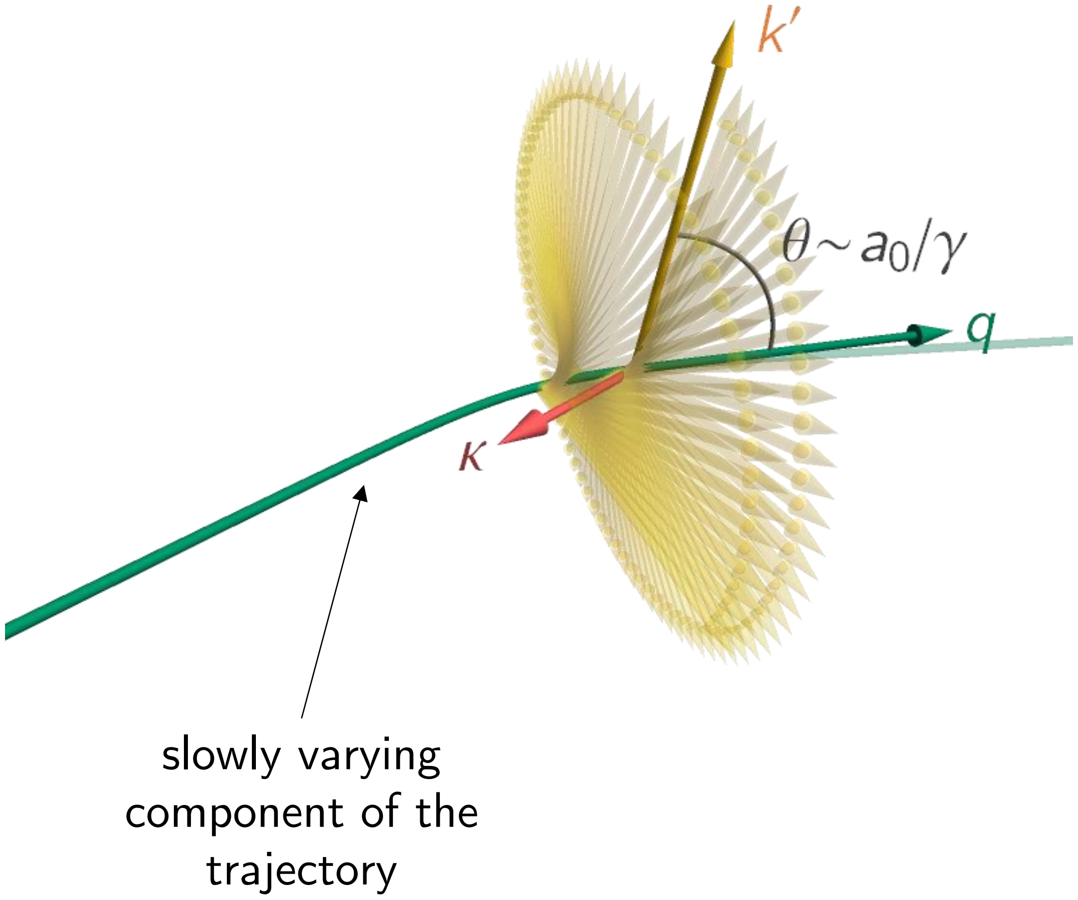
- For this to work well, the formation length of a photon emission event must be much smaller than the laser wavelength...
- ✓ if the field is strong and the emitted photon energy is not small.
- In the transition regime, we need to account for interference effects at the scale of the laser wavelength.

The locally monochromatic approximation



- Rate calculated for a plane EM wave with a slowly varying envelope (locally monochromatic approximation).
- Quantity that enters the rate is the quasimomentum $q^\mu = \langle \pi^\mu \rangle$, which is a cycle-averaged quantity, and the local parameters $\langle a^2 \rangle$ and $\eta = k.q/m^2$.
- Equation of motion is the relativistic ponderomotive force $\dot{\boldsymbol{q}} = -\frac{m^2}{2q^0} \boldsymbol{\nabla} \langle a^2 \rangle$

The locally monochromatic approximation



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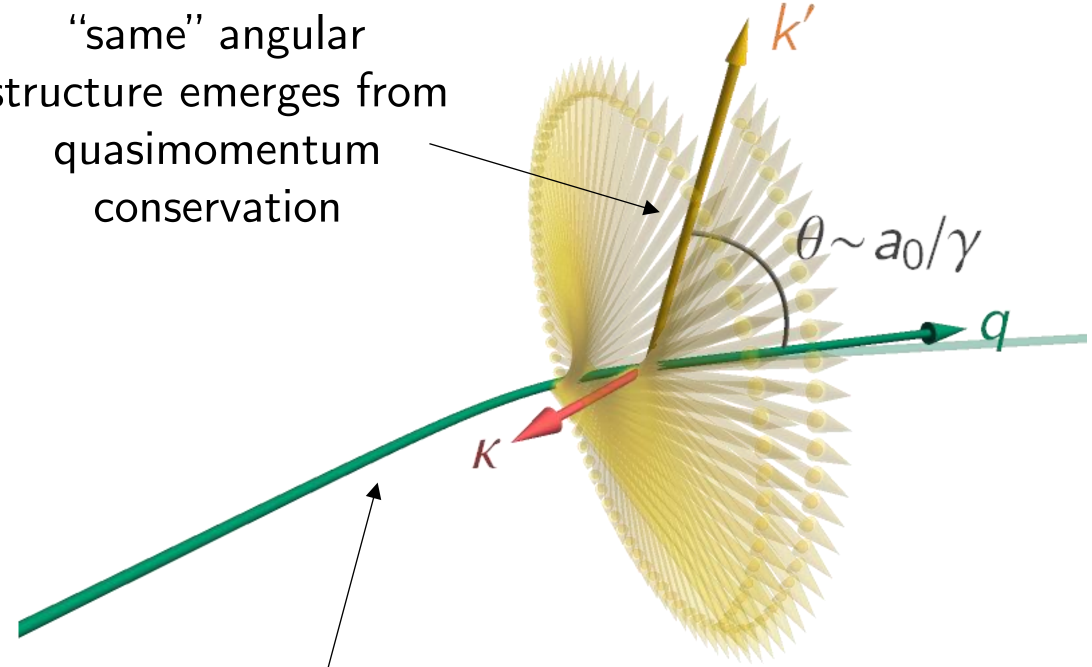
The locally monochromatic approximation

"same" angular structure emerges from quasimomentum conservation



slowly varying component of the trajectory

- Rate calculated for a plane EM wave with a slowly varying envelope (locally monochromatic approximation).
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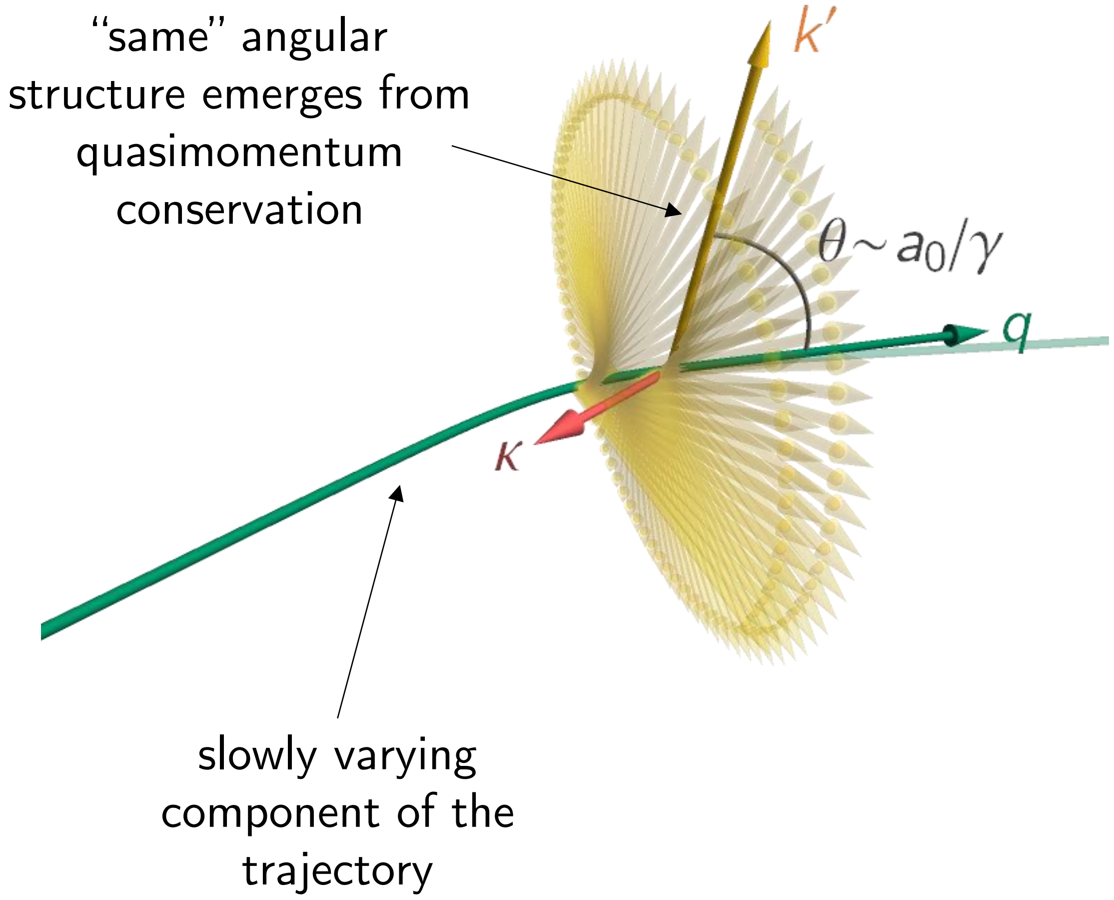
What if a_0 is not large?

The locally monochromatic approximation



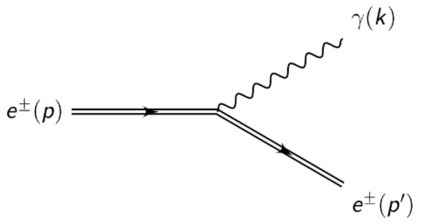
- Already used (if not named as such) in codes like NI (C. Bula/E144) and CAIN.
- Formalised in Heinzl, King and Macleod, PRA 102, 063110 (2020).
- Derived from plane-wave QED, combines a slowly varying envelope approximation and an expansion in a local phase.

LUXE's theory/simulation requirements

Electron + laser	Bremsstrahlung γ + laser	Electron + laser

Electron + laser

Nonlinear Compton scattering



Signals:

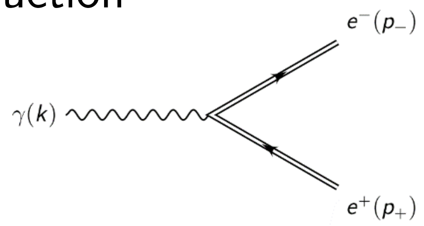
- Intensity dependence of Compton edges
- γ-photon angular profile

Needed:

- Photon emission rate

Bremsstrahlung γ + laser

Nonlinear Breit-Wheeler pair production



Signals:

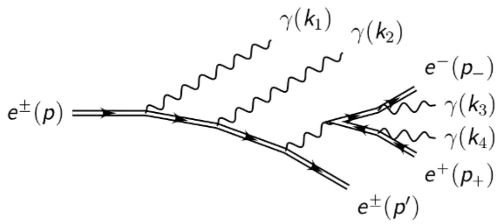
- Intensity dependence of positron yield

Needed:

- Pair creation rate, unpolarized γ photons

Electron + laser

Nonlinear trident pair creation



Signals:

- Intensity dependence of positron yield

Needed:

- Photon emission rate, γ-polarization resolved
- Pair creation rate, γ-polarization resolved

Simulations Q&A

Summary

- Code vs code:
  - Comparison of different codes (Ptarmigan, PIC), what they can or cannot do.
  - Why doesn't the LCFA work at $a_0 = 1$?
  - Why has no-one else implemented the LMA?
  - Is it possible to include the LMA in PIC?
  - How to simulate SFQED in crystals?

- Accuracy:
  - How accurate are our simulations (how can we even estimate this)? How can we benchmark the accuracy of approximations (e.g. LMA) in the nonperturbative regime, where few data exist (if any) and no reliable theoretical calculation exists?
  - Where do simulation tools really reach their limits and need testing?
  - If LUXE were to find significant disagreements with expectations, which part of the modelling would be first addressed?

Code vs code

Q: Comparison of different codes (Ptarmigan, PIC)?

$$\frac{\partial \phi_e}{\partial t} + \frac{\mathbf{p}}{\gamma m} \cdot \frac{\partial \phi_e}{\partial \mathbf{r}} - e\left(\mathbf{E} + \frac{\mathbf{p} \times \mathbf{B}}{\gamma m}\right) \cdot \frac{\partial \phi_e}{\partial \mathbf{p}} = - \phi_e \int w_{e \to e\gamma}(\mathbf{p}, \mathbf{q})\, \mathrm{d}^3\mathbf{q} + \int \phi_e' w_{e \to e\gamma}(\mathbf{p}', \mathbf{p}' - \mathbf{p})\, \mathrm{d}^3\mathbf{p}',$$

photon emission

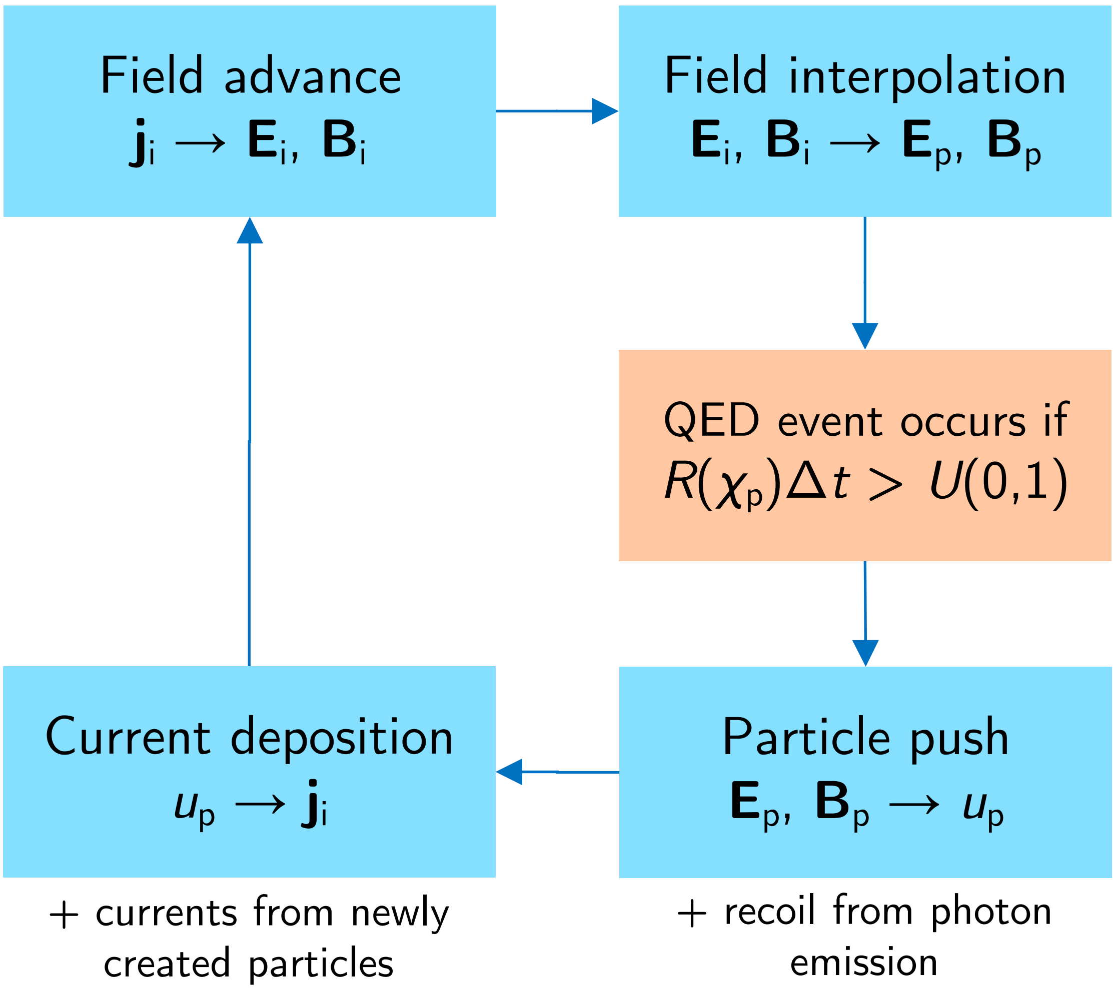
$$+ \int_0^1 \left[\phi_\pm \frac{dP^c}{d\epsilon'} + \phi_\gamma \frac{dP^b}{d\epsilon'} \right] d\epsilon$$

pair creation

Sokolov et al, PRL 105, 195005 (2010)
Elkina et al, PRSTAB 14, 054401 (2011)
Bulanov et al, PRA 87, 062110 (2013)

- *In LCFA mode*, Ptarmigan and PIC codes work in almost the same way, because they're solving almost the same problem.
- PIC codes don't have an equivalent of LMA mode.
- Subtle differences in implementation: Ptarmigan uses triple-differential rates, not single-differential. Spin not available, but polarization is.

Particle-in-cell codes + QED



- Particle-in-cell codes solve for the classical evolution of the electron (etc) distribution functions, as sampled by ‘macroparticles’.
- Probability rates for all QED processes integrated along macroparticle trajectory.
- Electrons recoil on photon emission, new electrons and positrons added on photon decay.

PIC codes that include SFQED processes

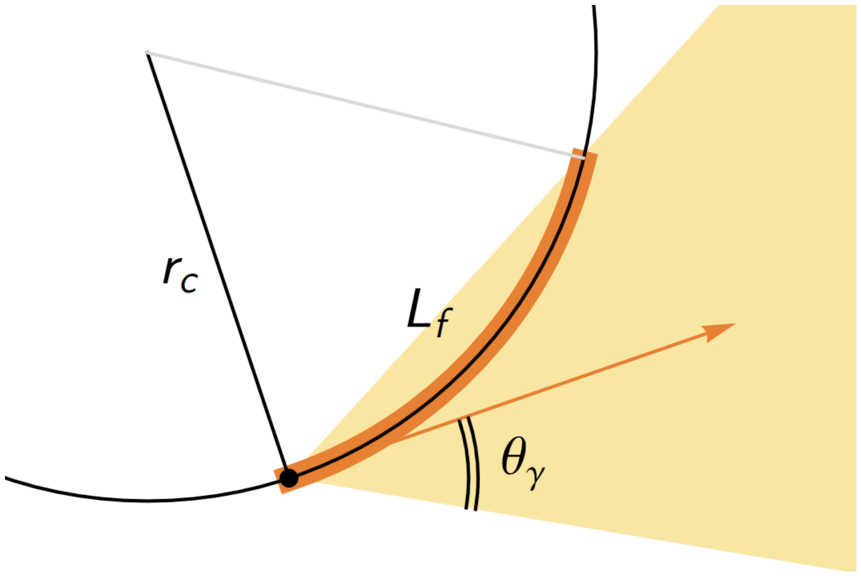
EPOCH | CALDER | Smilei :)

PICADOR | PIConGPU | WarpX

Osiris 4.0 | VLPL | QUILL

Code vs code

Q: Why doesn't the LCFA work at $a_0 = 1$?



$$\frac{L_f}{C} = \frac{1}{2\pi a_0}$$

- Interference.
- Formation length comparable in size to the laser wavelength.
- The electron "knows" about the oscillation of the background field.
- Undulator vs wiggler.

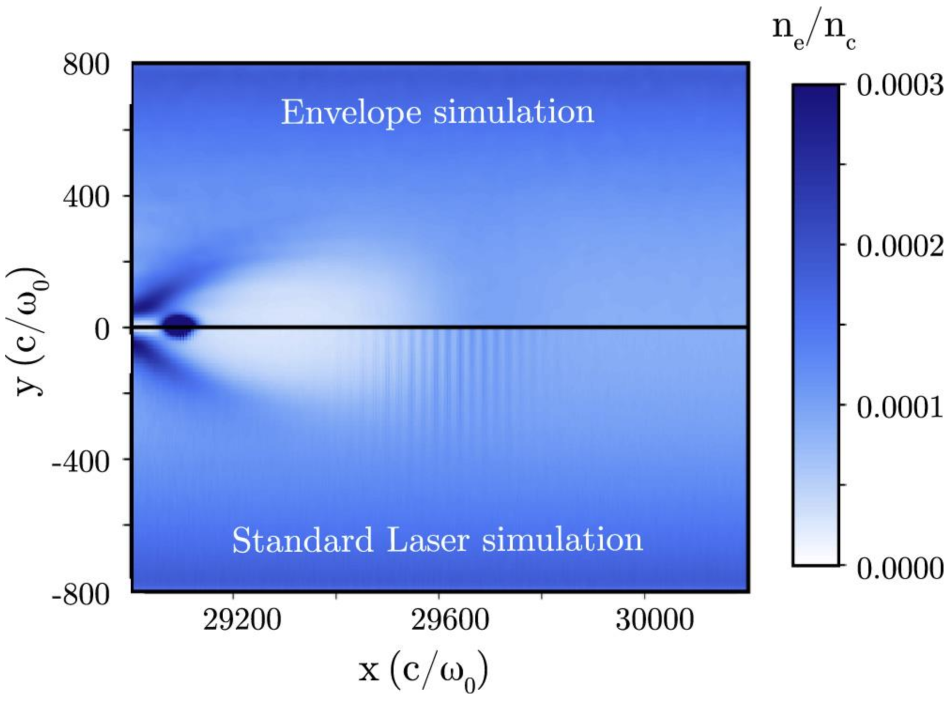
Code vs code

Q: Why has no-one else implemented the LMA?

- They have!
- NI [E144, see Appendix of Bamber et al, PRD 60, 092004 (1997)]
- CAIN [https://www-jlc.kek.jp/subg/ir/lib/cain21b.manual/main.html]
- Unclear how they propagate the particles between interactions (ballistically?)

Code vs code

Q: Is it possible to include the LMA in PIC?



from Massimo et al, PPCF 61, 124001 (2019)

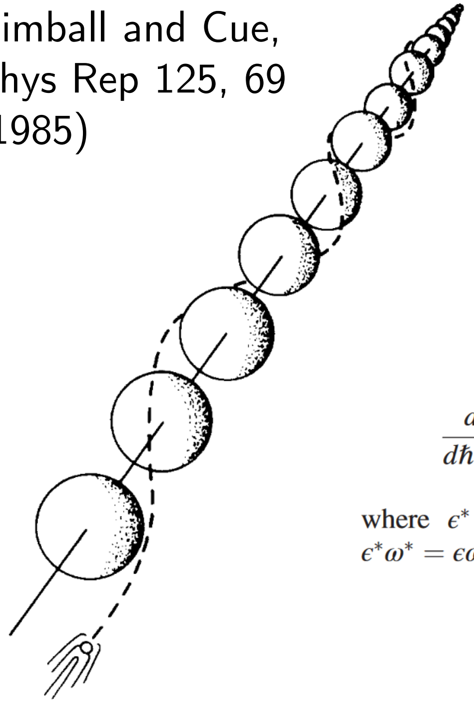
- Yes...
- ...but no.
- Envelope solvers solve the same (classical) equations of motion as Ptarmigan.
- Lightfront momentum must be large!

Simulations Q&A

Code vs code

Q: How to simulate QED effects in crystals?

Kimball and Cue, Phys Rep 125, 69 (1985)



$$\frac{d^2P}{d\hbar\omega\, d\Omega} = \frac{e^2}{4\pi^3}\left(\frac{\epsilon^{*2}+\epsilon^2}{2\hbar\omega\epsilon^2}|\mathbf{I}|^2 + \frac{\hbar\omega}{2\epsilon^2\gamma^2}|J|^2\right), \qquad (34)$$

where $\epsilon^* = \epsilon - \hbar\omega$ (with ω^* defined via the relation $\epsilon^*\omega^* = \epsilon\omega$) and I and J are given by

$$\mathbf{I} = \int_{-\infty}^{\infty} \frac{\boldsymbol{n}\times[(\boldsymbol{n}-\boldsymbol{\beta})\times\dot{\boldsymbol{\beta}}]}{(1-\boldsymbol{n}\cdot\boldsymbol{\beta})^2} e^{i\omega^*(t-\boldsymbol{n}\cdot\boldsymbol{r})}dt, \qquad (35)$$

$$J = \int_{-\infty}^{\infty} \frac{\boldsymbol{n}\cdot\dot{\boldsymbol{\beta}}}{(1-\boldsymbol{n}\cdot\boldsymbol{\beta})^2} e^{i\omega^*(t-\boldsymbol{n}\cdot\boldsymbol{r})}dt. \qquad (36)$$

Nielsen, Holtzapple and King, PRD 106, 013010 (2022)

- LCFA, of course.
- Define an equivalent a_0 using the oscillation frequency of a channelled positron as $6E_0^{1/2}$ [100 GeV].
- If multiplicity < 1 (fewer than one photon per electron on average), another option is Baier-Katkov, which assumes a classical trajectory. Patch together trajectories if multiplicity is larger...

Summary

- Code vs code:
  - Comparison of different codes (Ptarmigan, PIC), what they can or cannot do.
  - Why doesn't the LCFA work at $a_0 = 1$?
  - Why has no-one else implemented the LMA?
  - Is it possible to include the LMA in PIC?
  - How to simulate SFQED in crystals?

- Accuracy:
  - How accurate are our simulations (how can we even estimate this)? How can we benchmark the accuracy of approximations (e.g. LMA) in the nonperturbative regime, where few data exist (if any) and no reliable theoretical calculation exists?
  - Where do simulation tools really reach their limits and need testing?
  - If LUXE were to find significant disagreements with expectations, which part of the modelling would be first addressed?

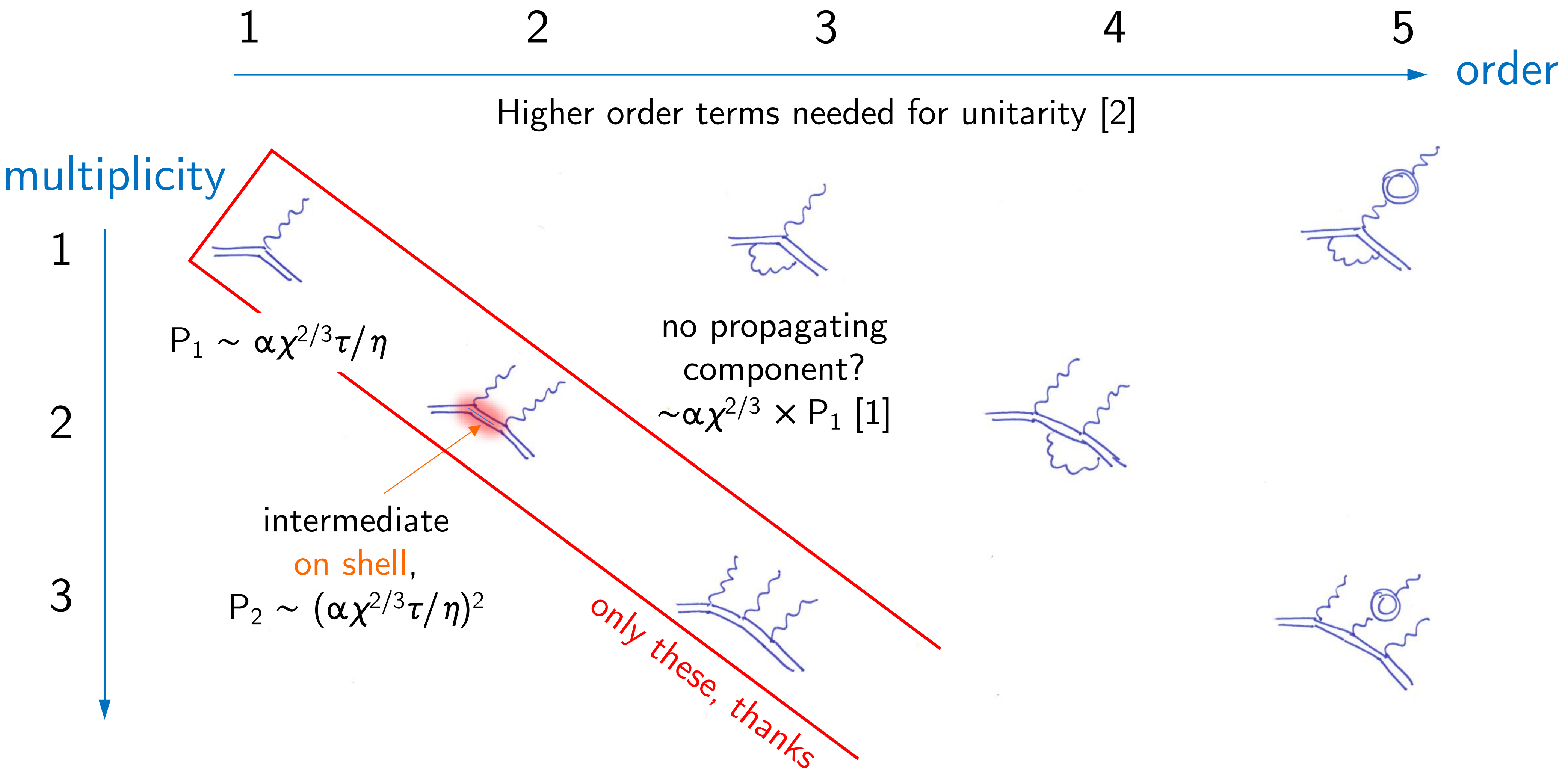
Accuracy

Q: How accurate are our simulations? How do we even estimate this?

- Verification: how well does a code reproduce the underlying theory.
- Size of missing terms?
  - Terms unknown, code does not compute an expansion.
- Argument based on asymptotics:
  - Plane wave? Diffraction angle small
  - LCFA? a_0 and $a_0{}^3/\chi$ large
  - LMA? Pulse duration large

- Compare where we can: single emission (or classical regime).
- Procedure:
  - Probability → mean number of photons.
  - Disable recoil to guarantee Poisson statistics.

Interaction with the radiation field



[1] Morozov, Narozhny and Ritus, JETP 53, 1103 (1981)
[2] Ilderton and Torgrimsson, PLB 725, 481 (2013); Heinzl, Ilderton and King, PRL 127, 061601 (2021)

Accuracy

Q: If LUXE were to find significant disagreements with expectations, which part of the modelling would be first addressed?

- In general, assumptions about collision parameters first, especially laser structure.
- Otherwise, it depends on the regime. At low a_0, theory is best constrained (perturbative), so plane wave + LMA there.
- At higher a_0, cascade approximation (propagation between events).

Summary

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Overview

A male ptarmigan in winter plumage

- Ptarmigan is a Monte-Carlo particle-tracking code that simulates the interaction between high-energy electron/photon beams and laser pulses.
- Designed to be accurate (and fast) across the full range of a_0.
- Single-particle, so collective interactions neglected, as well as feedback on the laser fields.

Physics coverage

Process	Polarization			Available modes		
	e^+/e^-	γ	laser	QED	classical	modified classical
Photon emission	averaged (initial), summed (final)	arbitrary	LP / CP	LMA / LCFA	LMA / LCFA	LCFA
Pair creation	summed	arbitrary	LP / CP	LMA / LCFA	n/a	n/a

- Fundamental processes included are: photon emission (NLC) and electron-positron pair creation (NLBW).
- All processes fully angularly resolved.
- Building blocks for higher-order processes, like EM showers.

Physics coverage

Process	Polarization			Available modes		
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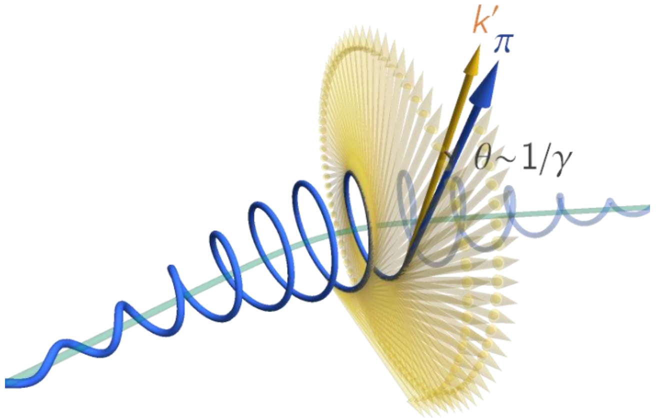
- LMA available for $a_0 \leq 20$ and $\eta = \chi/a_0 \leq 2$ [170 GeV @ λ = 800 nm]
- LCFA available for arbitrary χ.
- Classical radiation reaction also available (Landau-Lifshitz, including Gaunt factor if so desired)

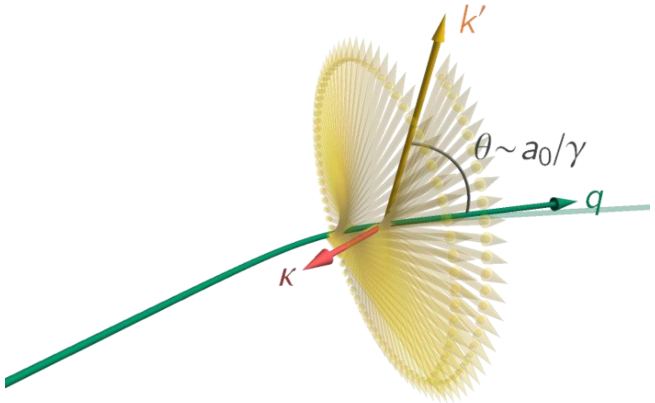
Approximations compared

LCFA:



- Locally constant field approximation
- Advantage: build arbitrary fields from slices of constant, crossed field.
- Disadvantage: no interference effects, does not work in transition regime.

LMA:

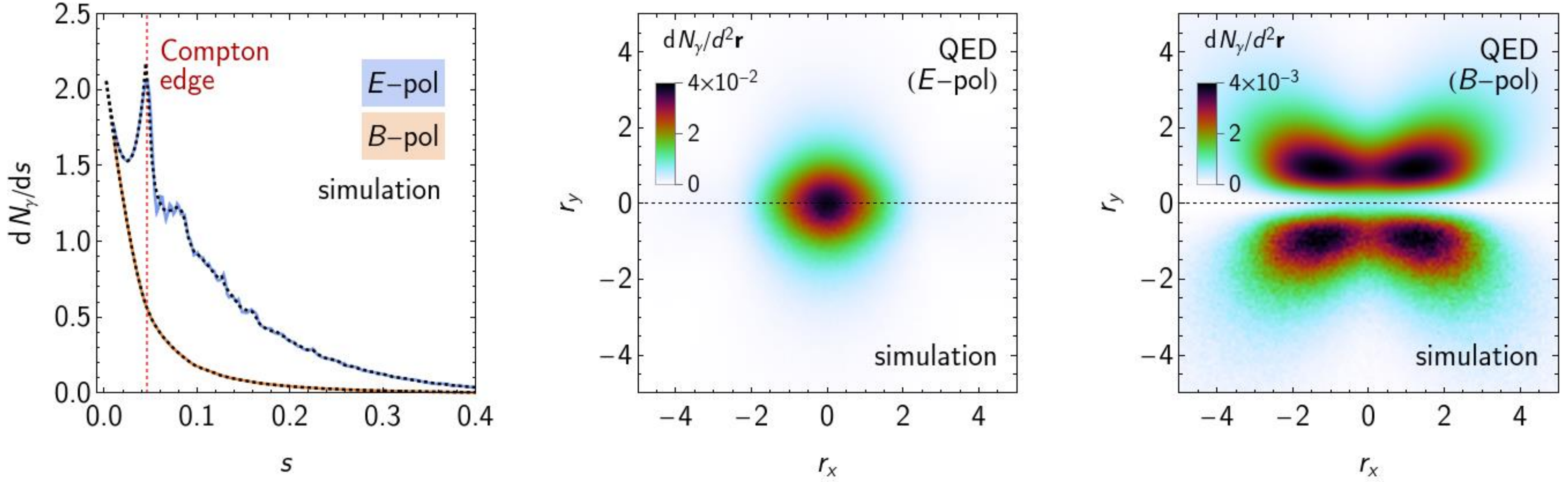


- Locally monochromatic approximation
- Advantage: includes wavelength-scale interference effects, works at all a_0.
- Disadvantage: background must be sufficiently "plane-wave-like", i.e. amplitude and frequency required.

Simulations with Ptarmigan

Benchmarking example

- $a_0 = 2.5$, under LMA:



- Photon spectra at fixed electron energy parameter $\eta = 0.1$ (8 GeV @ 800 nm laser wavelength). *E*-pol: photons polarized parallel to laser *E*; *B*-pol, perpendicular to *E*.

UNIVERSITY OF GOTHENBURG

Simulations with Ptarmigan

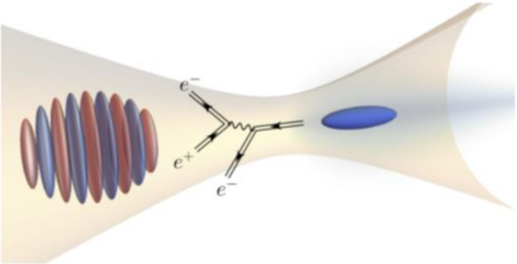
Access

README.md

Ptarmigan

OpenMPI build passing | MPICH build passing | release v1.3.2 | license Apache-2.0

Simulate the interaction between a high-energy particle beam and an intense laser pulse, including the classical dynamics and strong-field QED processes.



What's included

A summary of Ptarmigan's physics coverage can be found here.

Build

All of Ptarmigan's default dependencies are Rust crates, which are downloaded automatically by Cargo. Building the code in this case is as simple as running:

```
cargo build --release [-j NUM_THREADS]
```

- Open source and permissively licensed, available on Github (github.com/tgblackburn/ptarmigan).
- Documentation and example input files included, and more being added.
- MPI and HDF5 support available as opt-in features.
- Pull requests (bug fixed, additional features) always welcome!