

# Using Feynman's Tree Theorem to Evaluate Loop Integrals Numerically

Tobias Kleinschmidt

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In collaboration with W. Kilian



# Outline

- 1 Introduction
- 2 Cutting Loops
  - Feynman Tree Theorem
  - Renormalization and Regularization
  - Infrared Divergences
  - Threshold Singularities
- 3 Application to Bhabha Scattering
  - Cross Section Integration
  - Event Generation
- 4 Conclusions
  - Summary
  - Outlook

# Ingredients of NLO Calculations

- **Tree Graphs (real corrections) with  $n+1$  partons.**
  - ✓ Fully understood!
  - Several generators for creation of efficient matrix elements.  
e.g. O'Mega [Ohl et al., '01], Alpha [Caravaglios et al., '95], MadGraph [Stelzer et al., '03], Comix [Gleisberg, Höche '08]
  - Contain infrared soft and collinear divergences.
- Subtraction Terms
  - Cancel divergences in real corrections locally.
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  - Mainly used: [Catani, Seymour '96; Catani, Seymour, Dittmaier, Trocsanyi '02]
- Virtual Corrections to  $n$ -leg process
  - Contain... Problems!

Level of Complexity rises due to:

- Length of Expressions
- Complexity of Integrals
- IR divergences, internal singularities

Calculations very time consuming! (Not only computing time!)

➡ Aim at fully automated matrix element generation and event generation

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# Major Tools and Techniques for One Loop Calculations

## Feynman Diagram based methods

- Tensor reduction (PV) → set of basis integrals
- ✓ Scalar integrals known analytically
- ✗ Yields large expressions for coefficients
- ✗ can have delicate numerical stability
- ⇒ use modified reduction schemes, avoiding Gram determinants

GOLEM: Binoth, Guillet, Heinrich, Pilon, Reiter, ...

Denner, Dittmaier, ...

## Unitarity based methods

- Decompose Amplitude into scalar integrals and coefficients
- Coefficients are products of on-shell tree amplitudes, obtained by cutting techniques
- ✗ large expressions for coefficients, but...
- ✓ simpler than coefficients from PV-style reductions?
- ✓ P-algorithm ( $\tau \propto N^9$ , for N-gluon-amp)

Rocket: Ellis, Giele, Kunszt, Melnikov, Zanderighi

BlackHat: Bern, Dixon, Forde, Gleisberg, Kosower, Maitre,...

Helac-1Loop: van Hameren, Papadopoulos, Pittau,

Bevilacqua, Czakon, Worek...

- Fully numerical methods: Integrate over loop momentum/Feynman parameter
- ✓ No large expressions
- ✗ Complicated singularity structure
- ⇒ Sector Decomposition, Contour Deformation
- Anastasiou, Beerli, Daleo, Krämer, Nagy, Soper, ...
- ✗ Can again create large expressions

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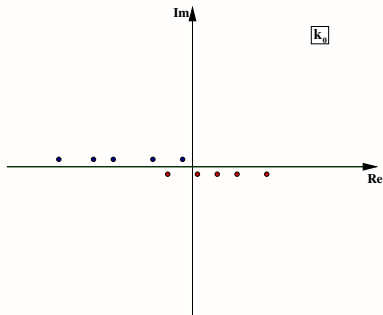
# Derivation of the Feynman Tree Theorem

- Integrand  $I(k)$  of a one-loop graph with loop momentum  $k$ :

$$I(k) = N(k) \prod_i F_i$$

with *Feynman* Green Functions  $F_i$  (t'Hooft-Feynman gauge):

$$F_i \equiv \frac{i}{(k + p_i)^2 - m_i^2 + i\epsilon}$$



- Partial fraction decomposition yields

$$F_i = \frac{i}{2E_i} \left( \frac{1}{k^0 - (-p_i^0 + E_i - i\epsilon)} - \frac{1}{k^0 - (-p_i^0 - E_i + i\epsilon)} \right), \quad E_i = \sqrt{(\vec{k} + \vec{p}_i)^2 + m_i^2}.$$

- Idea: Replace *Feynman* Green functions  $F_i$  by *advanced* ones  $A_i$ :

$$A_i = \frac{i}{2E_i} \left( \frac{1}{k^0 - (-p_i^0 + E_i + i\epsilon)} - \frac{1}{k^0 - (-p_i^0 - E_i + i\epsilon)} \right)$$

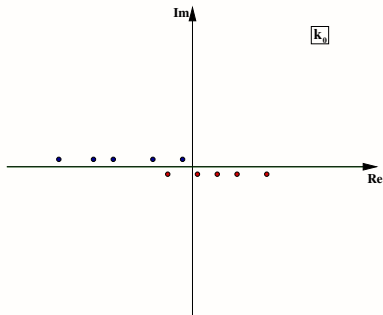
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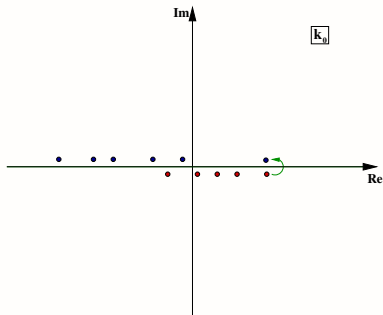
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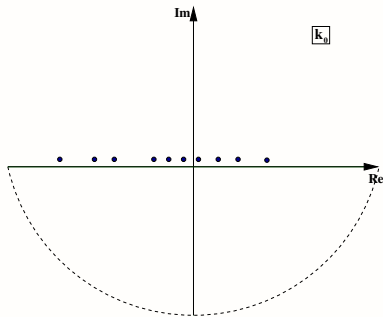
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# Derivation of the Feynman Tree Theorem

- Difference of *Feynman* and *advanced* Green function:

$$\Delta_i^l \equiv F_i - A_i = \frac{i}{2E_i} \left( \frac{1}{k^0 - (-p_i^0 + E_i) + i\epsilon} - \frac{1}{k^0 - (-p_i^0 + E_i) - i\epsilon} \right)$$

$$\stackrel{\epsilon \rightarrow 0}{=} \frac{2\pi}{2E_i} \delta(k^0 - (-p_i^0 + E_i)).$$

$\Rightarrow \Delta_i^l$  sets momentum  $k + p_i$  on-shell with positive energy component  $E_i$ .

$$0 = \int N(k) \prod_i^n A_i$$

- Replacing  $A_i$  with  $F_i - \Delta_i^l$  yields:

## Feynman Tree Theorem (FTT)

$$0 = \int N(k) \left[ F \cdots F - \sum \Delta^l F \cdots + \sum \Delta^l \Delta^l F \cdots - \dots + (-1)^n \sum \Delta^l \cdots \Delta^l \right]$$

Acta. Phys. Polon. **24** (1963) 697

- Recent interest: Brandhuber ea.[hep-th/0510253], Catani ea.[0804.3170]
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- Make use of identity:

$$\frac{1}{x-a \pm i\epsilon} = \mathcal{P} \frac{1}{x-a} \mp i\pi\delta(x-a)$$

- Rewrite Feynman Green function  $F_i$ :

$$F_i = P_i + \frac{1}{2}\Delta_i^l + \frac{1}{2}\Delta_i^u$$

$$P_i = \mathcal{P} \frac{i}{(k+p_i)^2 - m_i^2}$$

$$\Delta_i^u = \frac{2\pi}{2E_i} \delta(k^0 - (-p_i^0 - E_i))$$

- Replace any  $F_i$  in subleading terms of FTT:

## Feynman Tree Theorem - Improved Version

$$\begin{aligned} \int I(k) &= \int N(k) [\Delta_1^l P_2 \cdots P_n + P_1 \Delta_2^l P_3 \cdots P_n + \dots + P_1 \cdots P_{n-1} \Delta_n^l] \\ &\quad + \int N(k) \sum_{\substack{\text{perm.} \\ U+L \geq 2}} C_{LUP} \Delta^{lL} \Delta^{uU} P^P, \\ C_{LUP} &= \frac{1}{2^{L+U}} \left(1 - (-1)^L\right) \end{aligned}$$

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Leading terms: 
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- Performing  $k_0$  integration,  $\Delta_i^l$  act as *opening* or *cutting* the loop:

- Momentum  $k + p_i$  is set on-shell
- Numerator of cut propagator is product of wave functions, summed over all internal states
- Loop integral is replaced by phase space integral

$$(\not{k} + \not{p}_i + m) = \sum_{\lambda} u_{\lambda}(k + p_i) \bar{u}_{\lambda}(k + p_i),$$

$$-g_{\mu\nu} \rightarrow \sum_{\sigma} \epsilon_{\mu}^*(k + p_i; \sigma) \epsilon_{\nu}(k + p_i; \sigma)$$

$$\int \frac{d^4 k}{(2\pi)^4} = \int \frac{d^3 k}{(2\pi)^3 2E_i}$$



Loop corrections for a  $2 \rightarrow n$  process can be computed by considering all possible  $2 + 1 \rightarrow n + 1$  tree graphs with an additional incoming and outgoing on-shell particle. A phase space integration over the additional particles' momenta has to be performed.

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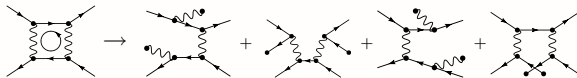
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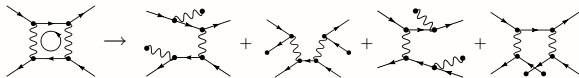
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$$(\not{k} + \not{p}_i + m) = \sum_{\lambda} u_{\lambda}(k + p_i) \bar{u}_{\lambda}(k + p_i);$$

$$-g_{\mu\nu} \rightarrow \sum_{\sigma} \epsilon_{\mu}^{*}(k + p_i; \sigma) \epsilon_{\nu}(k + p_i; \sigma)$$

$$\int \frac{d^4 k}{(2\pi)^4} = \int \frac{d^3 k}{(2\pi)^3 2E_i}.$$



Loop corrections for a  $2 \rightarrow n$  process can be computed by considering all possible  $2 + 1 \rightarrow n + 1$  tree graphs with an additional incoming and outgoing on-shell particle. A phase space integration over the additional particles' momenta has to be performed.

## Advantages

- Tree graphs simple to generate automatically,
- Phase space integrations *under control* for up to 8 final state particles.
- Phase space integration over additional particles can be performed simultaneously with integrations over external particle momenta.

Make method ideally suited for implementation in existing matrix element and event generator frameworks.

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- 1 Renormalization and regularization scheme
- 2 Treatment of infrared divergences
- 3 Treatment of threshold singularities

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- Born Level  $\Rightarrow$  Loop Level: Relation bare  $\Leftrightarrow$  physical parameters broken
  - Add renormalization constants to Lagrangian (also absorb UV divergences)
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  - Fix by renormalization conditions
- Use *on-shell* renormalization scheme [Ross and Taylor, '73]:

$$\begin{aligned} \text{Re } i\Gamma_{\alpha\beta}^{(2)}(-p, p)\Phi^\beta(p)\Big|_{p^2=m^2} &= 0 & \Gamma^{(3)}(p_i, \lambda)\Big|_{p_i^2=m^2} &= \lambda_0^3 \\ \text{Res } (-\Gamma^{(2)}(p))^{-1}\Big|_{\not{p}=m, p^2=m^2} &= 1 & \Gamma^{(4)}(p_i, \lambda)\Big|_{p_i^2=m^2} &= \lambda_0^4 \end{aligned}$$

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[Bogoliubov, Parasiuk, Hepp, Zimmermann, '57,'70]

1PI n-point function:

$$\hat{\Gamma}^n(p_1, \dots, p_n) = \Gamma^n(p_1, \dots, p_n) - T \circ \Gamma^n(p_1, \dots, p_n)$$

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- Virtual one loop cross section:

$$\begin{aligned}\sigma_v^{(1)} &= \Phi \int d\Pi_n 2 \operatorname{Re}(\mathcal{M}^{\text{Born}}(\mathcal{M}_n^{\text{loop}} + \mathcal{M}_{n,\text{CT}}^{\text{loop}})^*) \\ &= \Phi \int d\Pi_n \int \frac{d^3k}{(2\pi)^3} 2 \operatorname{Re}(\mathcal{M}_n^{\text{Born}}(\mathcal{M}_{n+1}^{\text{Tree}} + \mathcal{M}_{n+1,\text{CT}}^{\text{Tree}})^*)\end{aligned}$$

3-dim integral UV convergent. ✓

- Infrared divergent terms in  $\mathcal{M}_{n+1}^{\text{Tree}}$  and  $\mathcal{M}_{n+1,\text{CT}}^{\text{Tree}}$ . Compensated by addition of real emission graphs [Kinoshita, '63; Lee, Nauenberg, '64]

$$\sigma_{\text{re}}^{(1)} = \Phi \int d\Pi_n \int \frac{d^3k}{(2\pi)^3 2E_k} |\mathcal{M}_{n+\gamma}^{\text{Born}}|^2$$

Contains implicit  $\delta$ -function conserving overall momentum.  
 $\Rightarrow$  Need approximation for soft real emission diagrams.

The diagram shows a self-energy loop on a propagator (a circle with two external lines) equal to the difference of three diagrams. Each of the three diagrams on the right has a self-energy loop on a propagator, but with a cut line (indicated by a dashed line) through the loop. The first cut is on the left side, the second on the top side, and the third on the right side.

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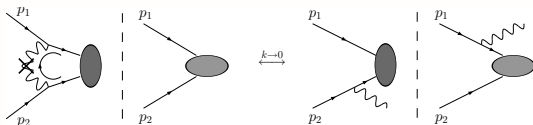
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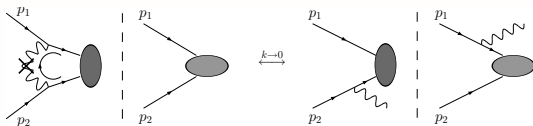
- Virtual IR-divergence arises solely from cut of massless particle.
- In limit  $k \rightarrow 0$ , expressions for cut loop and real emission compensate each other.
- Two equivalent approaches:
  - Project  $n + \gamma$  amplitude on  $n$ -particle phase space.
  - Modify tree graph of cut massless propagator.

→ In the following (2nd approach):

$$\mathcal{M}_{n,\gamma\text{-cut}}^{\text{Tree}} \rightarrow \mathcal{M}_{n,\gamma\text{-cut}}^{\text{Tree}} \theta(|\vec{k}| - E_s), \quad E_s: \text{soft cut}$$

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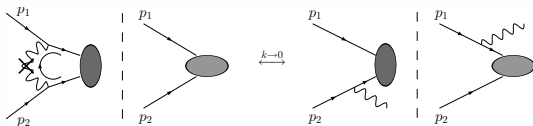
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### 3. Threshold Singularities

- Propagators of tree graphs can become singular in parts of integration region.

$$P_j = \frac{i}{(k + p_j)^2 - m_j^2} = \frac{i}{\left(k^0 - (-p_j^0 + E_j)\right) \left(k^0 - (-p_j^0 - E_j)\right)}$$

- After cutting propagator  $P_i$ , one of the two factors in  $P_j$  can get zero:

$$(p_j^0 - p_i^0) + (E_i \mp E_j) = 0$$

- Vanishing of first factor corresponds to coincidence of original poles in lower half plane.  
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## Construction of Fix Functions

- In rest frame of  $p_{ji}$ , peak of threshold singularity is spherical:

$$I(\mathbf{k}') \propto \frac{1}{\mathbf{k}' - \mathbf{k}_s}, \quad \mathbf{k}_s = \frac{\lambda^{\frac{1}{2}}(p_{ji}^0, m_i^2, m_j^2)}{2|p_{ji}^0|}$$

- Problematic for integration algorithms.
- Idea: Subtract zero from integrand:

$$\frac{\text{Res}(k'_s)}{\mathbf{k}' - \mathbf{k}_s}$$

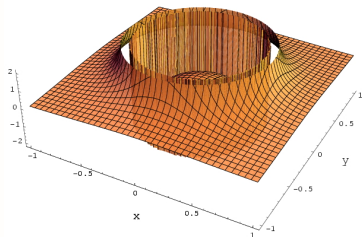
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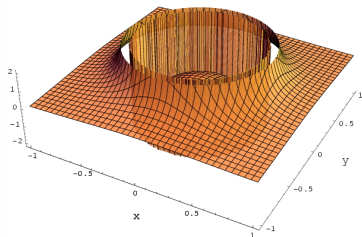
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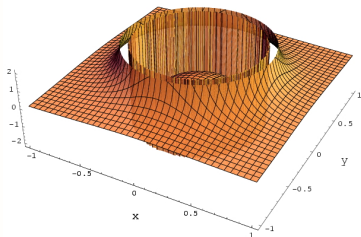
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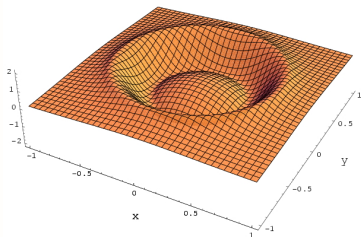
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# Overlapping Peaks

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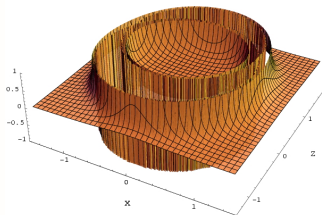
$$\frac{f(r, \theta, \phi) - f(r, \theta, \phi)|_{r'=b}}{(r'(r, \theta, \phi) - b)}$$

- Equals derivative with respect to  $r'$  in the limit  $r' \rightarrow b$ .
- 1st term corresponds to original integrand; 2nd resembles fix function.
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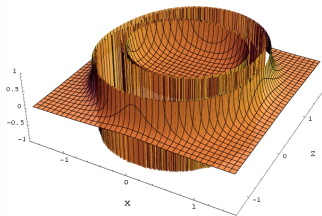
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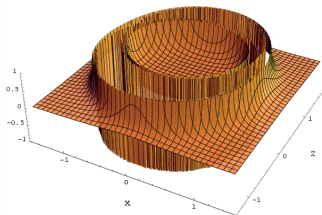
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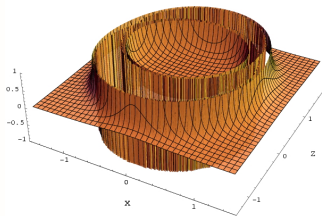
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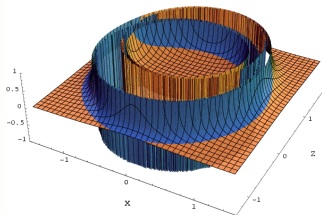
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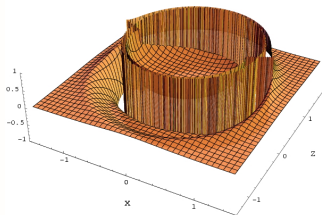
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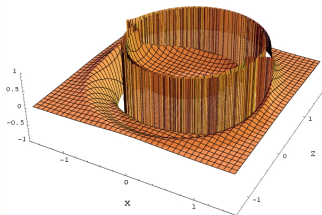
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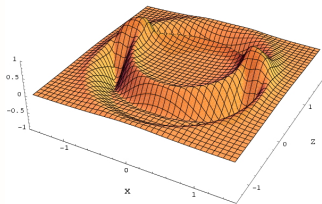
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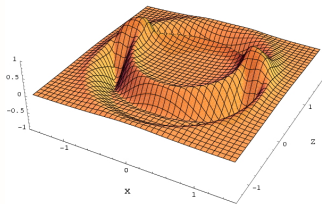
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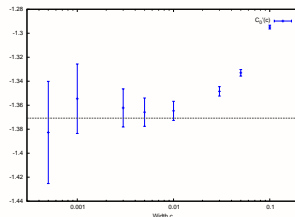
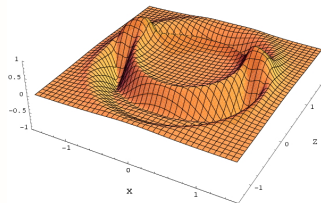
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- 1 Introduction
- 2 Cutting Loops
  - Feynman Tree Theorem
  - Renormalization and Regularization
  - Infrared Divergences
  - Threshold Singularities
- 3 Application to Bhabha Scattering**
  - Cross Section Integration
  - Event Generation
- 4 Conclusions
  - Summary
  - Outlook

# Bhabha Scattering

## Application of FTT to QED Bhabha Scattering at NLO as Proof of Principle

- Includes 10 loop graphs, 2pt, 3pt and 4pt functions.
- Test subtraction scheme for UV/IR divergences and internal singularities
- Two different scales:  $m_e \approx 500 \text{ keV}$ ,  $\sqrt{s} \approx 500 \text{ GeV}$

⇒ Compare with automated packages; FeynArts/FormCalc [Hahn ea, '98]

## Recipe

### In Mathematica

- Create loop graphs with FeynArts/FormCalc. No tensor reduction.
- Create subtraction graphs
- Cut loops and add fix functions
- Create Channels for Multi Channel Routine

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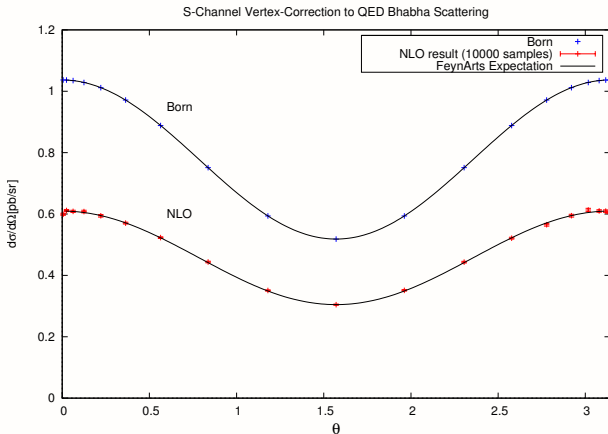
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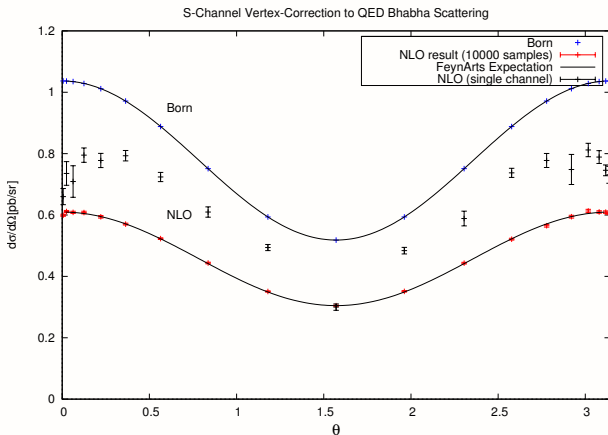
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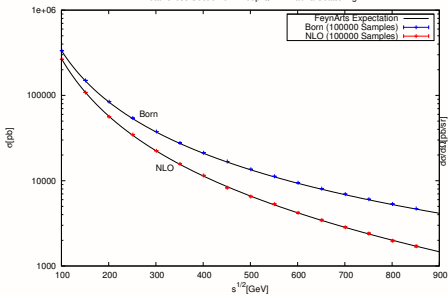
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Total Cross Section of 1-Loop QED Bhabha Scattering



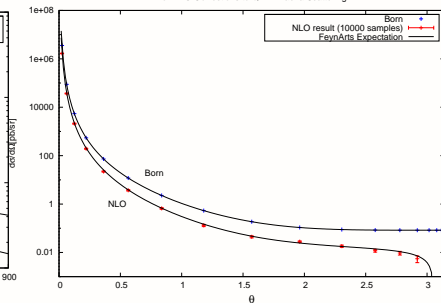
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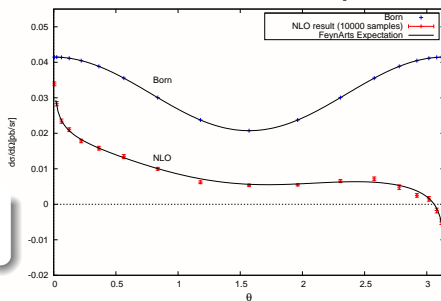
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Full NLO Corrections to QED Bhabha Scattering



S-Channel Corrections to QED Bhabha Scattering



# Monte Carlo Event Generation

## Include NLO by using FTT

- Additional 3 inclusive variables  $k_i$  from phase space integral over additional particles in tree graphs
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  - ⇒ Expect gain in computation speed compared to (semi-)analytical methods.

## Negative Weights

- Integrand not positive definite
- Need to incorporate events with negative weights
  - Accept event if:

$$r \leq \frac{|w_i|}{w_{\max}^{\pm}} \quad w_{\max}^{\pm} = \max(|w_{\max}|, |w_{\min}|)$$

- Assign additional flag ( $\pm 1$ ) to event, dependent on sign of  $w_i$
- Expectation value, error:

$$\langle n_i \rangle = \langle n_i^+ \rangle - \langle n_i^- \rangle \quad s_i = \sqrt{\langle n_i^+ \rangle + \langle n_i^- \rangle}$$

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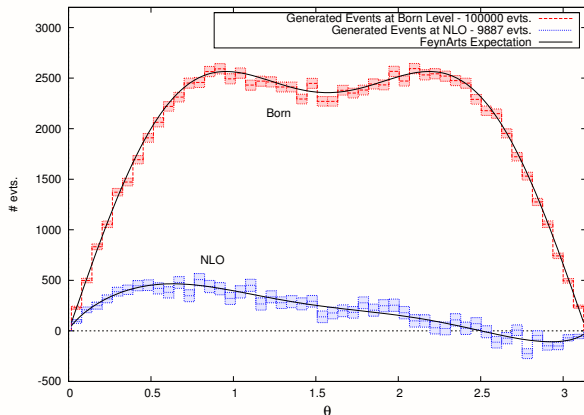
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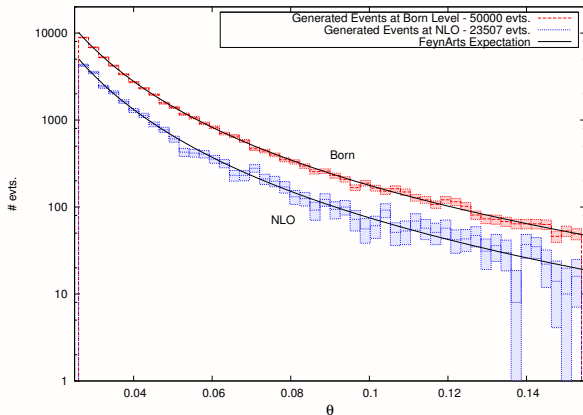
## Results - S Channel



- $\sigma_{\text{Born}}^{\text{tot}} = 0.34744(29)\text{pb}$
- $\text{eff}_{\text{Born}} = 66\%$
- $\mathcal{L} = 290\text{fb}^{-1}$

- $\sigma_{\text{NLO}}^{\text{tot}} = 0.03434(91)\text{pb}$
- $\text{eff}_{\text{NLO}}^{\text{p+n}} = 1.8\%$
- $\text{eff}_{\text{NLO}}^{\text{hist}} = 0.14\%$

## Results - Full Process in Forward Region



- $\sigma_{\text{Born}}^{\text{tot}} = 5981.3(3.3)\text{pb}$

- $\text{eff}_{\text{Born}} = 65\%$

- $\sigma_{\text{NLO}}^{\text{tot}} = 2812(24)\text{pb}$

- $\text{eff}_{\text{NLO}}^{\text{p+n}} = 3.0\%$

- $\text{eff}_{\text{NLO}}^{\text{hist}} = 0.8\%$

# Conclusions

## Summary

- Presented Method for computation of loop diagrams from tree graphs.  
⇒ allows fully numerical evaluation in matrix element/event generator framework
- Simple prescription for cancellation of UV-, IR-, internal singularities
- Proof of principle: Application to Bhabha scattering
- No further manipulations necessary  
⇒ Level of complexity rises solely due to increasing number of terms

## Outlook

- Extension to full Standard Model
- Implementation in event generator package
- Far future: Extension to two loops

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$pp \rightarrow VV \text{ jet}$	$t\bar{t}H$ , new physics
$pp \rightarrow t\bar{t}b\bar{b}$	$t\bar{t}H$
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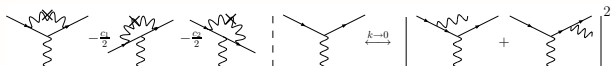
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- **However:** *on-shell* renormalization scheme; no one loop corrections to external on-shell particles.
- The corresponding infrared divergences of real emission graphs are compensated by subtraction terms of vertex corrections:



→ Additional prescription for BPHZ subtraction graphs for (photonic) vertex corrections: Divide in half and align momentum of (charged) particle with initial incoming and outgoing particle, respectively.

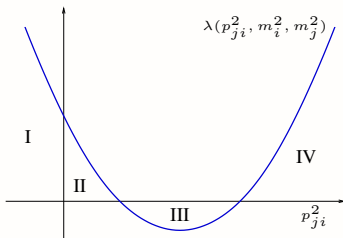
# Conditions for Singularities

- Four different regions for  $p_{ji}^2 = (p_j - p_i)^2$ .

Separated by  $p_{ji}^2 = 0$  and nodes of kinetic function  $\lambda$ :

$$\lambda(x, y, z) = x^2 + y^2 + z^2 - 2xy - 2xz - 2yz$$

$$\lambda(p_{ji}^2, m_i^2, m_j^2) = 0 \rightarrow p_{ji}^2 = (m_j \pm m_i)^2$$



Region	Occurrence	Cancellation in Sum
I	always	✓
II	dep. on loop momentum	✓
III	never	—
IV	always	✗

- Singularities appear if  $p_{ji}^2 > (m_i + m_j)^2$ . Production threshold of the two corresponding real particles.  
 $\Rightarrow$  Canceled by fix functions
- Amplitude gets imaginary part; covered by higher order terms in FTT.

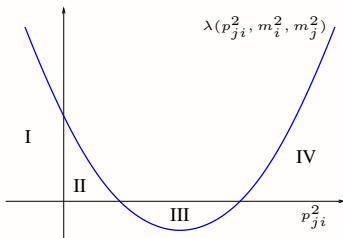
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# Coordinate Mappings

- In Fortran:

- Use single channel integration routine of VAMP [Ohl, '99]
- Map spherical coordinates on unit hypercube:

$$\begin{array}{rcl}
 r & = & a \left( \frac{1}{1-x_1} - 1 \right) \\
 \cos \theta & = & b - (b+1) \left( \frac{b-1}{b+1} \right)^{x_2} \\
 \phi & = & 2\pi x_3
 \end{array}
 \quad (x_1, x_2, x_3) \in [0, 1]^3$$

- Scaling factor  $a$ ; interesting region spread over wide parts of integration interval
- Jacobian  $\left| \frac{d \cos \theta}{dx_2} \right|$  cancels collinear peak:

$$I(k) \propto \frac{1}{(b - \cos \theta)}$$

$$b = \frac{\sqrt{s}}{\sqrt{s - 4m_e^2}}$$

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# WHIZARD: Phase Space Integration

- Matrix elements are complicated and vary over orders of magnitude
  - ⇒ Uniform phase space sampling yields no result
  - ⇒ No single parameterization allows for mapping the function into a constant
- **Solution:** Multi-channel parameterization with mappings and parameterizations adapted to Feynman diagram structure
  - \* WHIZARD: Improve by VEGAS adaptation within each channel
- What does this mean in practice?
  - WHIZARD has to find the *important* channels: The Feynman diagrams which have the strongest peaks ⇒ correspond to good parameterizations
  - WHIZARD has many degrees of freedom to adapt:
    - The optimal binning of each integration dimension (10 – 50)
    - This is needed for each integration dimension (10 – 20)
    - The optimal relative weight of each channel (10 – 1000)
  - ⇒  $10^3 - 10^6$  degrees of freedom have to self-optimize
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