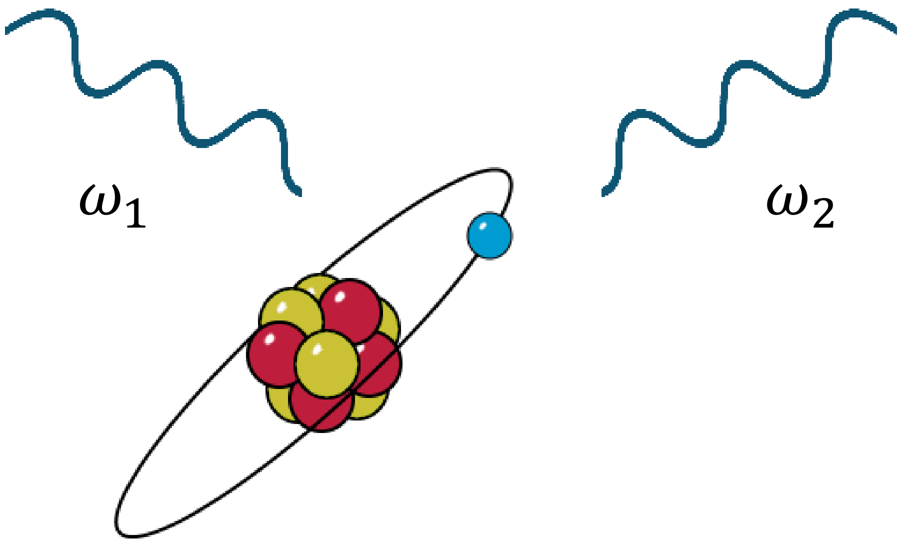
Coulomb Corrections to Delbrück Scattering

Jonas Sommerfeldt, FAIRNESS, 27.05.2022

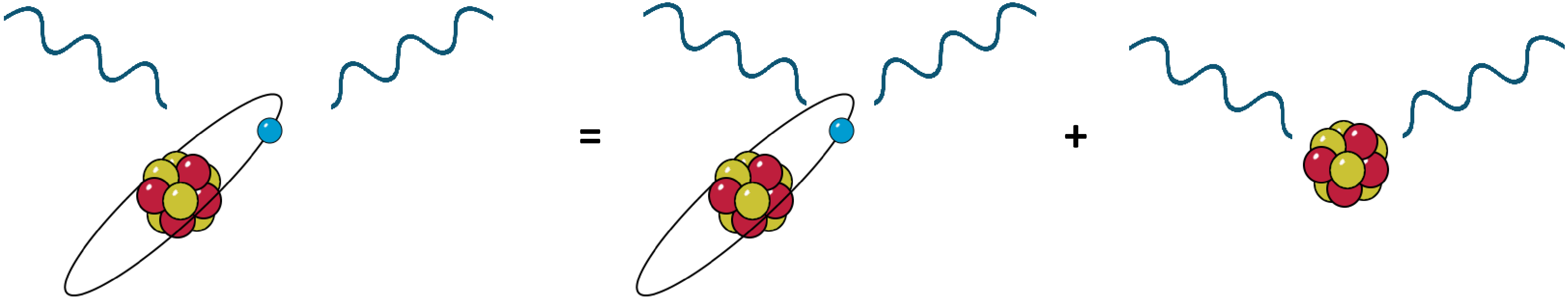
Elastic Photon Scattering



$$\omega_1 = \omega_2 = \omega$$

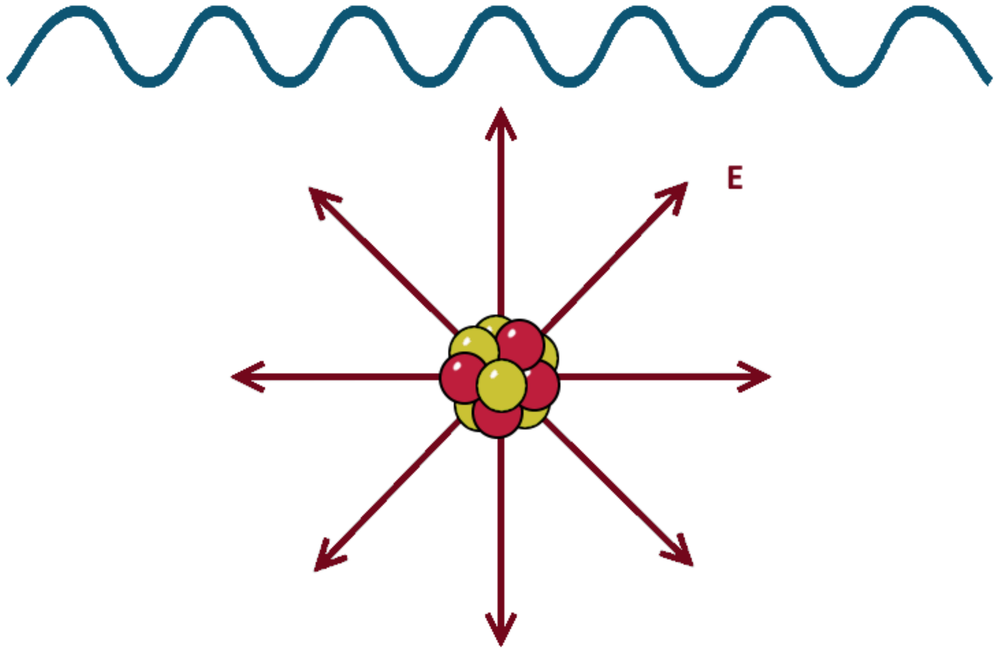
https://photon-science.desy.de/

Elastic Photon Scattering



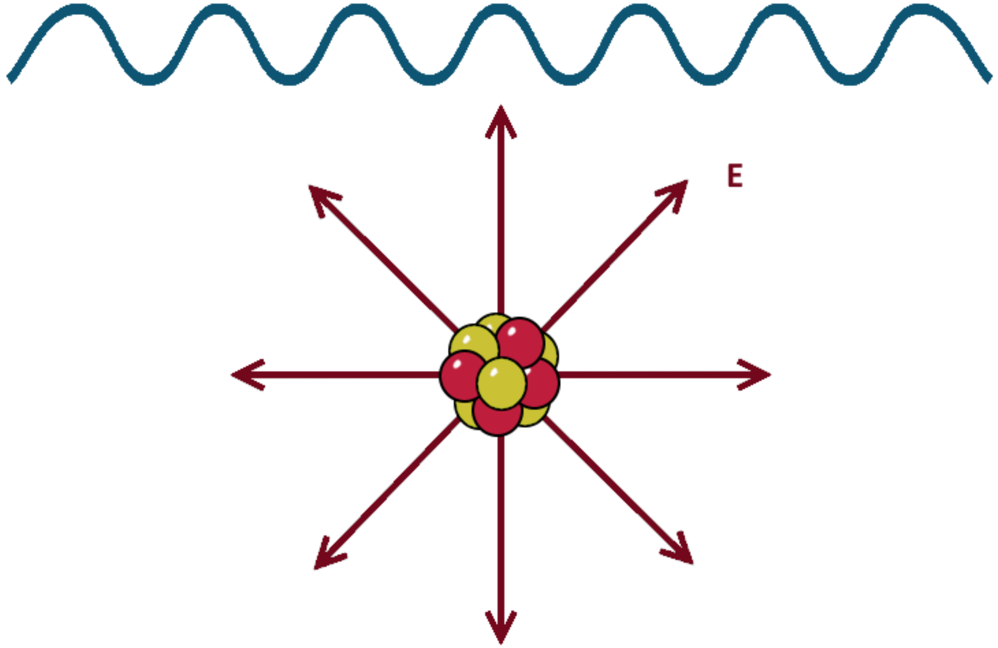
Elastic Photon Scattering | Rayleigh | Nuclear Compton

Delbrück Scattering

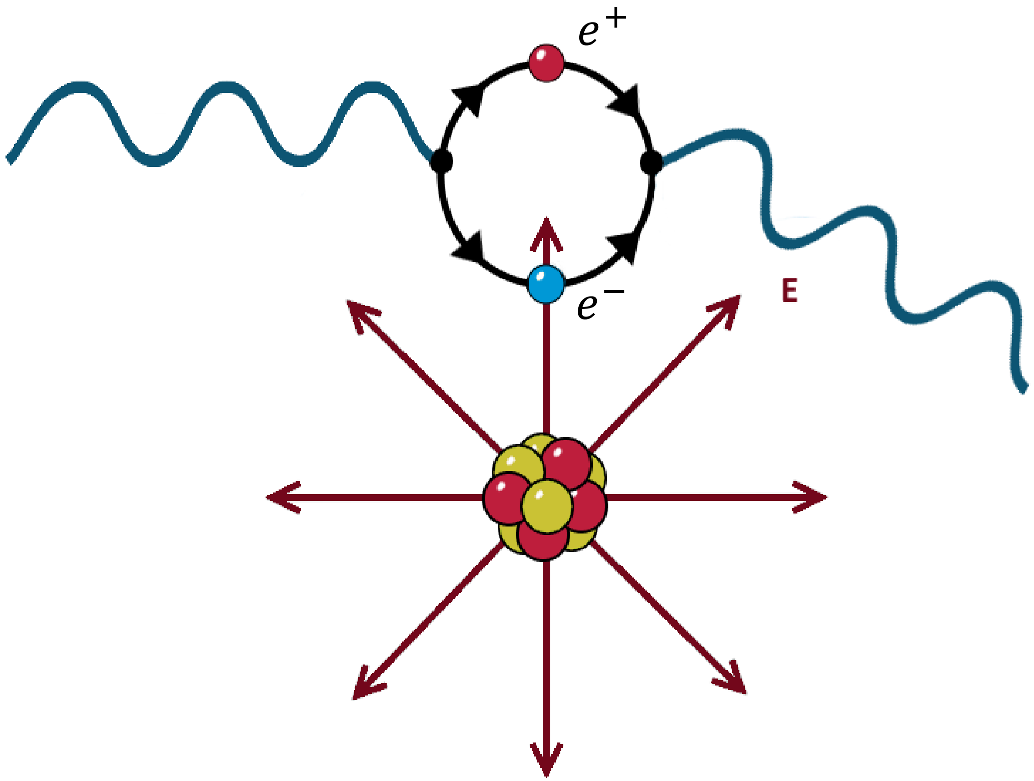


Classical electrodynamics: linear

Delbrück Scattering

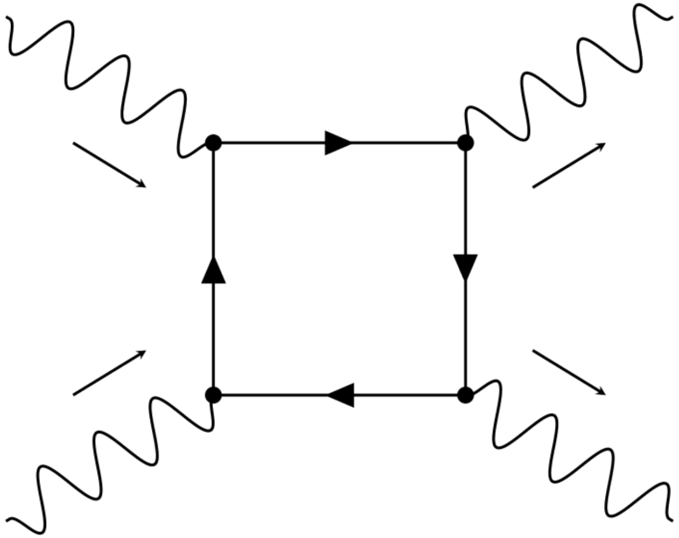


Classical electrodynamics: linear

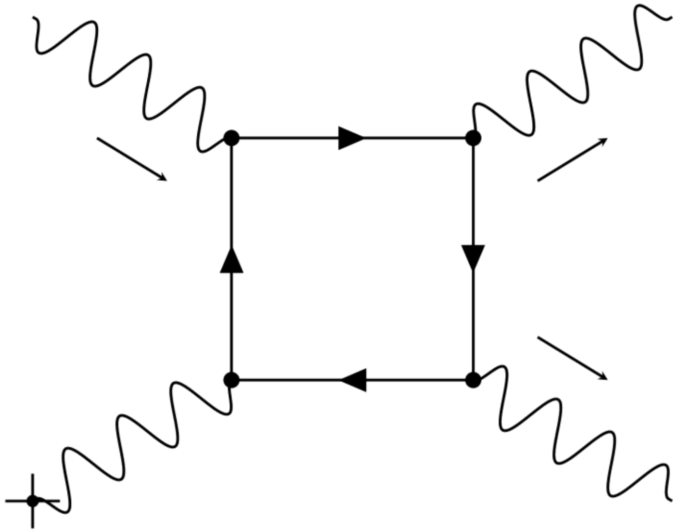


Quantum electrodynamics: non-linear

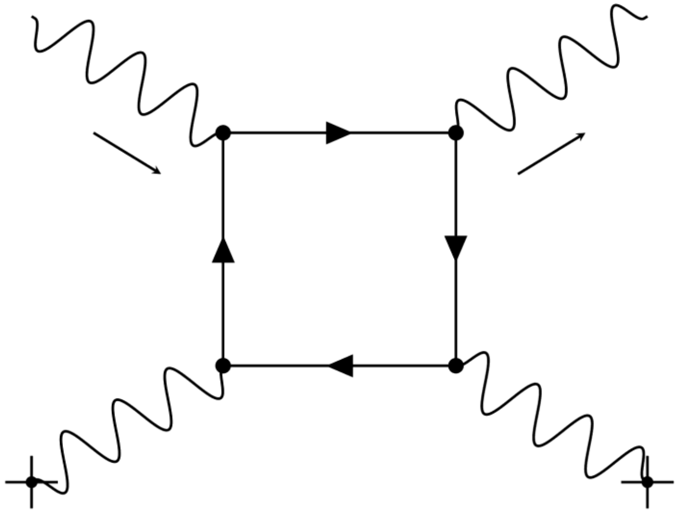
Non-linear QED processes



Light-by-light scattering
$\sim\alpha^2$

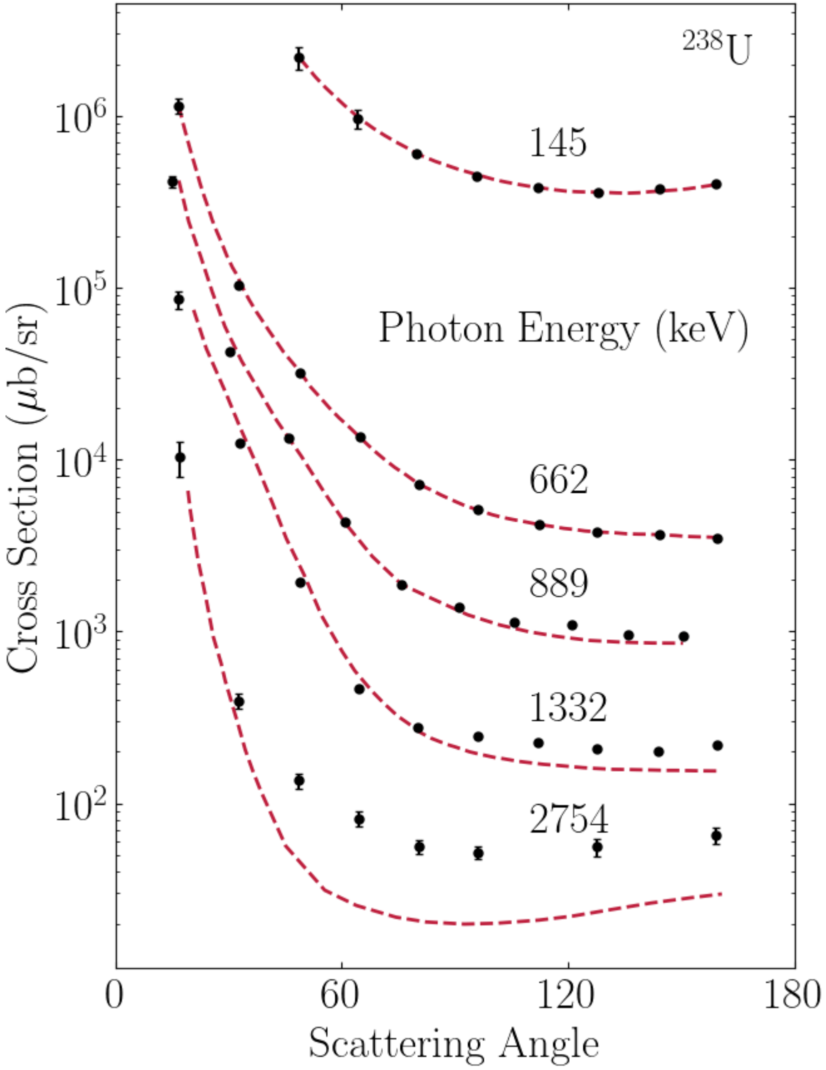


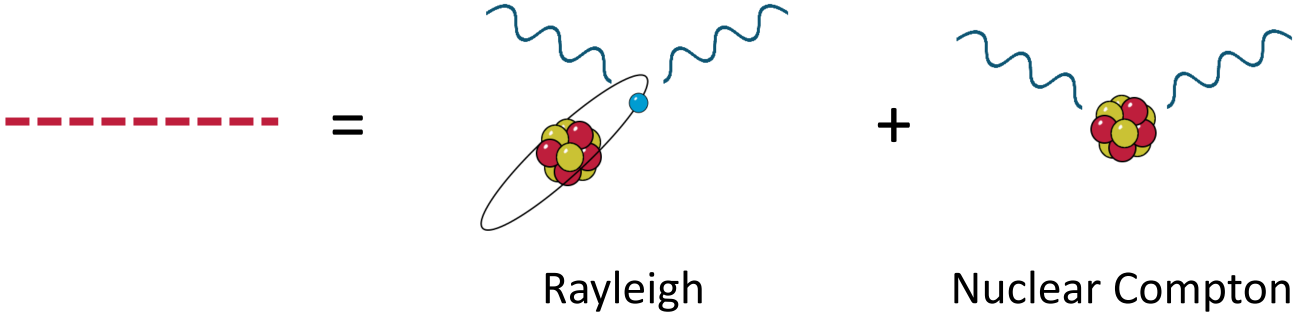
Photon splitting
$\sim\alpha^{3/2}(\alpha\mathrm{Z})$



Delbrück scattering
$\sim\alpha(\alpha Z)^2$

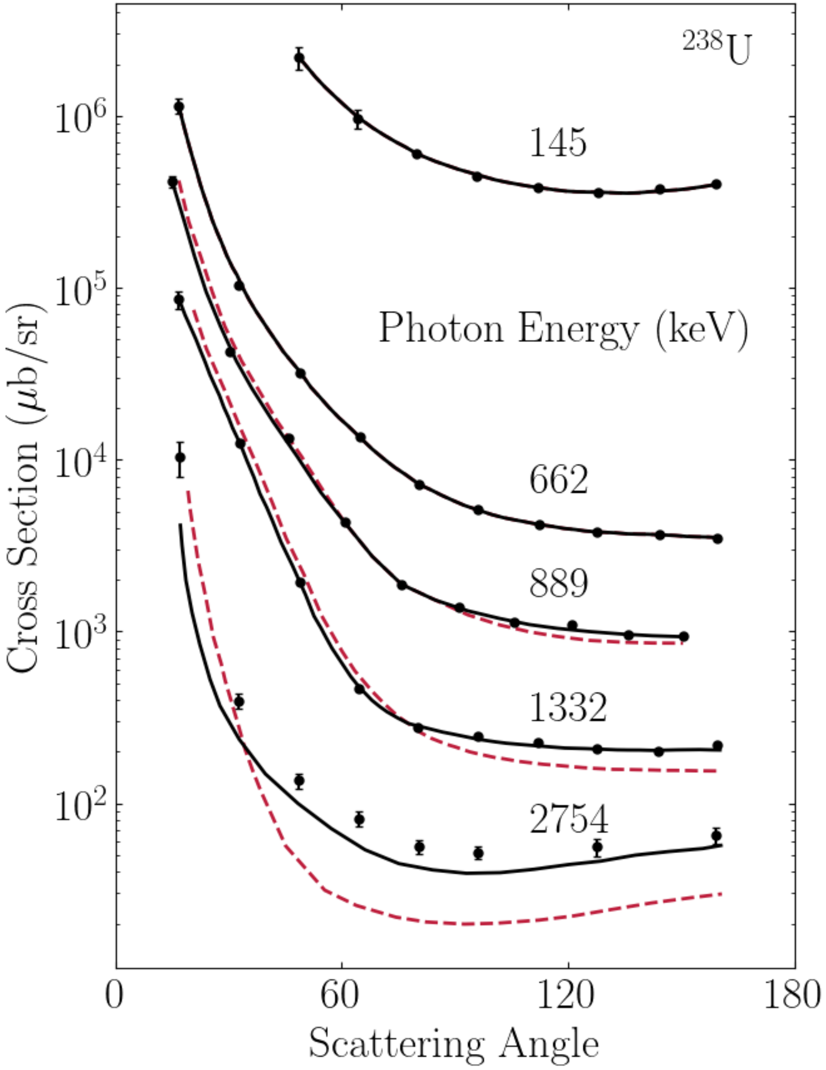
Experimental Observation of Delbrück Scattering



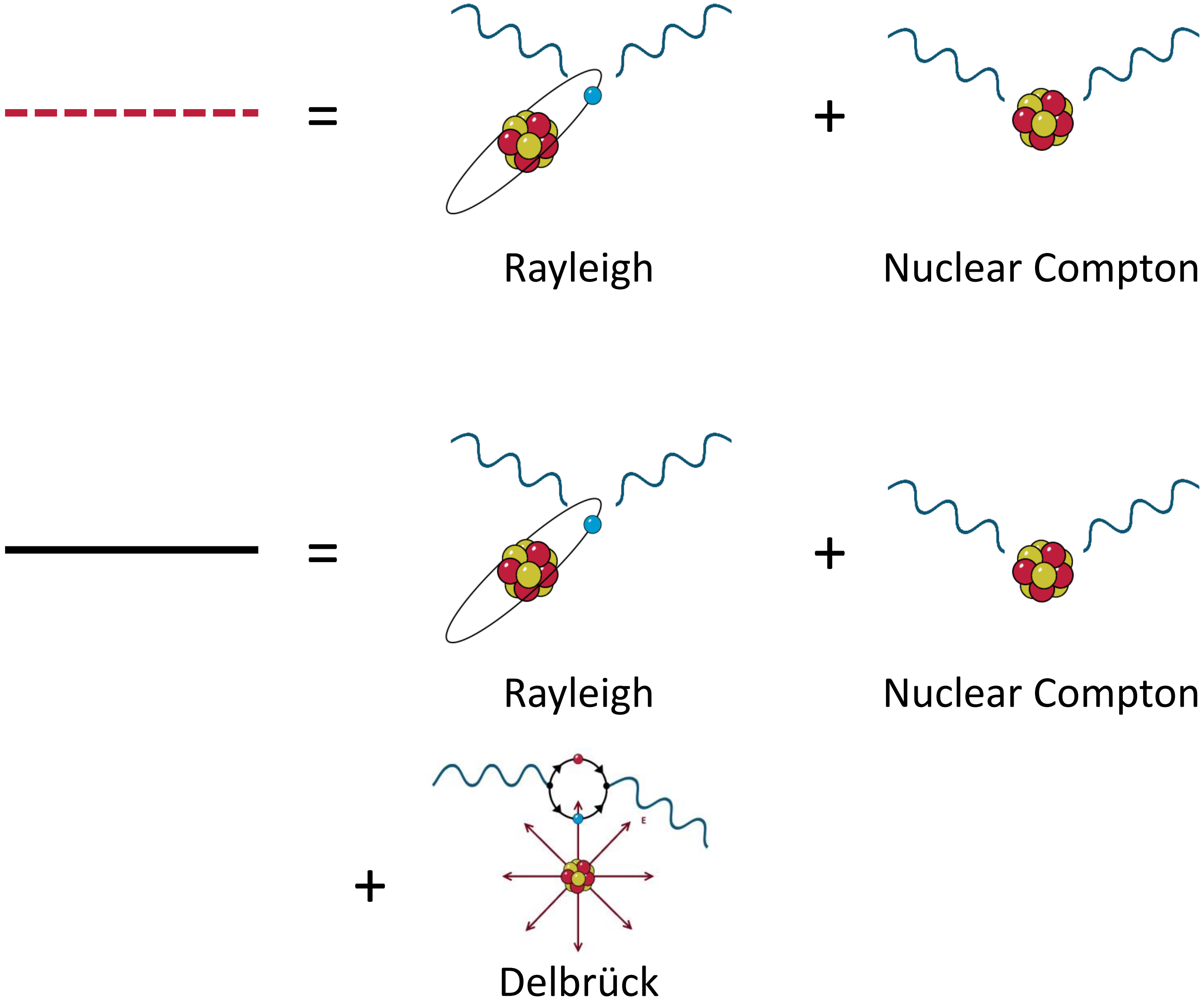


W. Mückenheim et al., J. Phys. G: Nucl. Phys 6, 1237-1250 (1980)
M. Schumacher, Radiat. Phys. Chem. 56, 101 (1999)

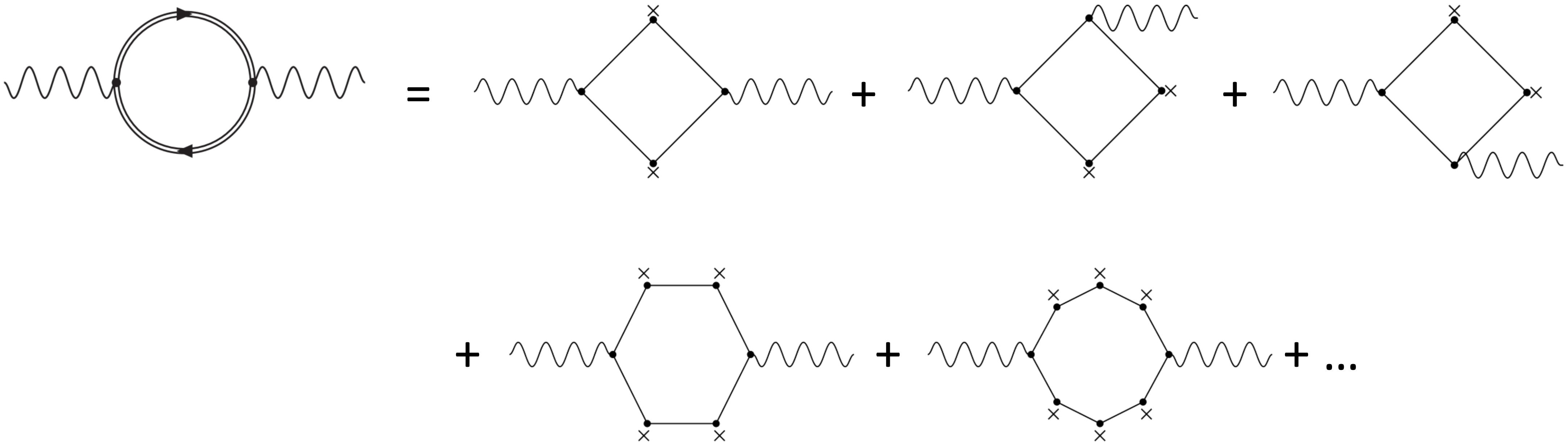
Experimental Observation of Delbrück Scattering



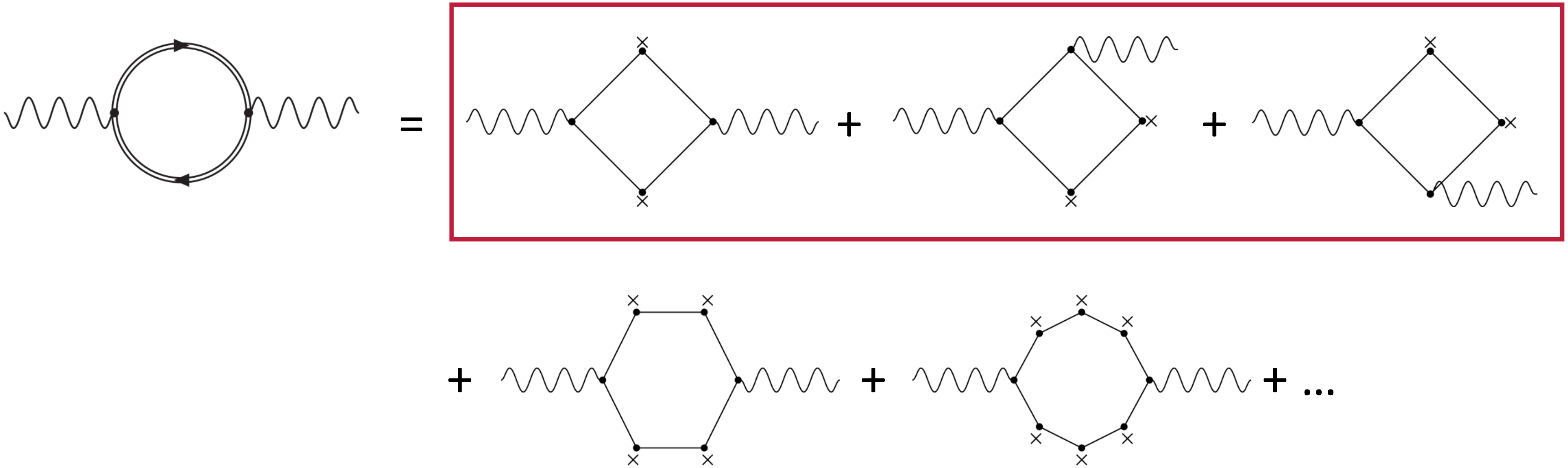
W. Mückenheim et al., J. Phys. G: Nucl. Phys 6, 1237-1250 (1980)
M. Schumacher, Radiat. Phys. Chem. 56, 101 (1999)



Full Delbrück Scattering Diagram



Full Delbrück Scattering Diagram

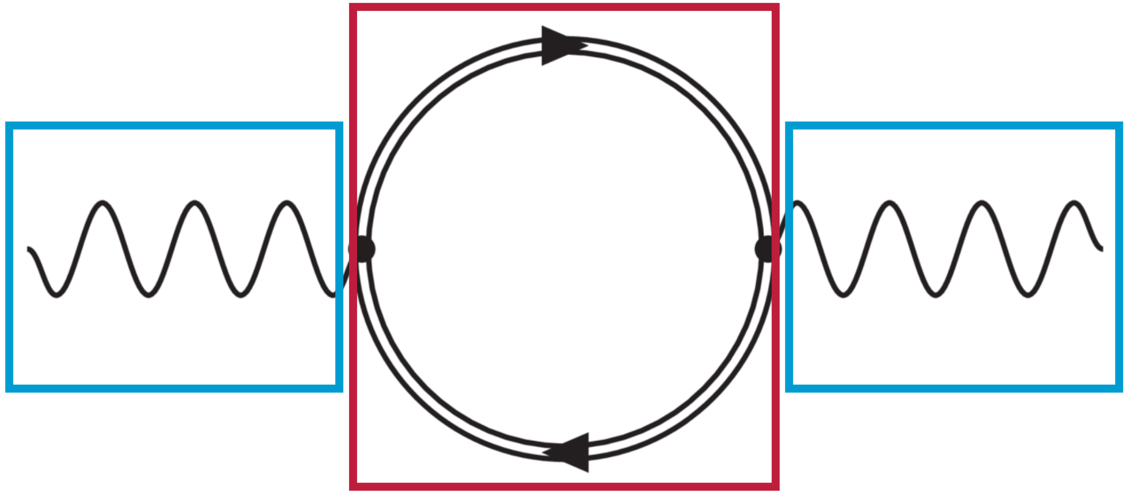


Theoretical values were obtained using the lowest-order Born approximation:

$\Rightarrow$ Contributions beyond $(\alpha Z)^2$ are neglected

$\Rightarrow$ Experiment and theory disagree for large nuclear charges

Amplitude for Delbrück Scattering

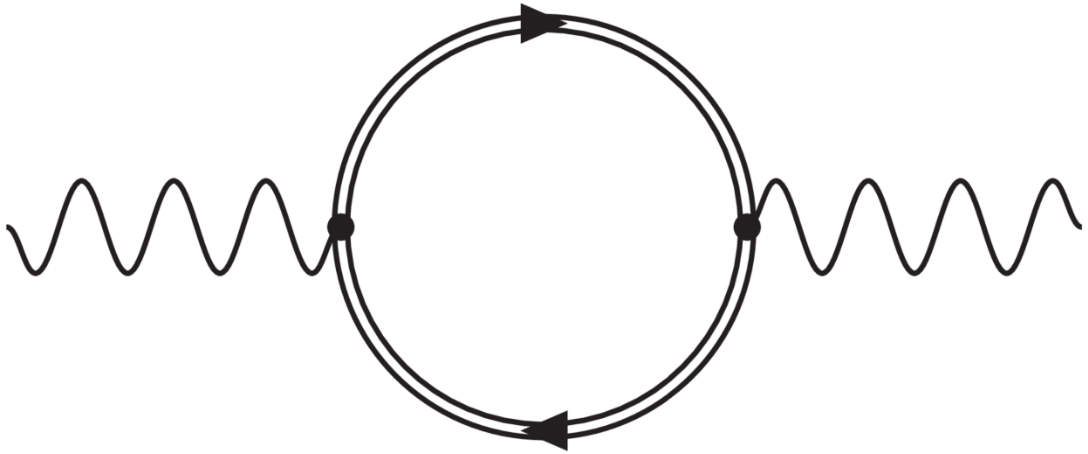


Electron-photon interaction operator

Electron Green's function

$$M = 2i\alpha \int_{-\infty}^{\infty} \mathrm{d}z \int_{-\infty}^{\infty} \mathrm{d}z' \int \mathrm{d}^3 x_1 \int \mathrm{d}^3 x_2 \mathrm{Tr}\left[\boxed{\hat{R}(\boldsymbol{x_1}, \boldsymbol{k_1}, \lambda_1)} \boxed{G(\boldsymbol{x_1}, \boldsymbol{x_2}, z)} \boxed{\hat{R}(\boldsymbol{x_2}, \boldsymbol{k_2}, \lambda_2)} \boxed{G(\boldsymbol{x_2}, \boldsymbol{x_1}, z')} \right] \delta(\omega + z - z')$$

Amplitude for Delbrück Scattering



$$M = 2i\alpha \boxed{\int_{-\infty}^{\infty} \mathrm{d}z \int_{-\infty}^{\infty} \mathrm{d}z'} \boxed{\int \mathrm{d}^3x_1 \int \mathrm{d}^3x_2} \mathrm{Tr}\left[\hat{R}(\boldsymbol{x_1}, \boldsymbol{k_1}, \lambda_1) \quad G(\boldsymbol{x_1}, \boldsymbol{x_2}, z) \quad \hat{R}(\boldsymbol{x_2}, \boldsymbol{k_2}, \lambda_2) \quad G(\boldsymbol{x_2}, \boldsymbol{x_1}, z') \right] \boxed{\delta(\omega + z - z')}$$

Energy integral & Spatial integrals

=> 7 dimensional integral

Multipole Expansion

We make a multipole expansion of the electron Green's function:

$$G(\boldsymbol{x}_2, \boldsymbol{x}_1, z) = \sum_{\kappa\mu} \frac{1}{w_\kappa} [\Theta(r_2 - r_1) F_{\kappa,\infty}(\boldsymbol{x}_2, z) F^\dagger_{\kappa,0}(\boldsymbol{x}_1, z) + \Theta(r_1 - r_2) F_{\kappa,0}(\boldsymbol{x}_2, z) F^\dagger_{\kappa,\infty}(\boldsymbol{x}_1, z)]$$

And the electron-photon interaction operator:

$$R(\boldsymbol{x}, \boldsymbol{k}, \lambda) = \boldsymbol{\alpha} \cdot \boldsymbol{\epsilon}_\lambda e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \sqrt{2\pi} \sum_{PLM} i^L \sqrt{2L+1} (i\lambda)^P D^L_{M\lambda}(\hat{\boldsymbol{k}}) \boldsymbol{\alpha} \cdot \boldsymbol{a}^P_{LM}$$

=> The angular integrals can be solved **analytically**

Delbrück Amplitude

What remains is a sum over all multipole components

$$M = \sum_{\kappa\mu} \sum_{\kappa'\mu'} \sum_{P_1 L_1 M_1} \sum_{P_2 L_2 M_2} I(\omega, Z, P_1, L_1, M_1, P_2, L_2, M_2, \kappa, \mu, \kappa', \mu', \hat{k}_1, \hat{k}_2)$$

Where the only non-trivial part of the calculation are integrals of the type

$$K = \int_{-\infty}^{\infty} \mathrm{d}z' \int_{-\infty}^{\infty} \mathrm{d}z \; \delta(\omega + z - z') \int_0^{\infty} \mathrm{d}r_2 \; g(r_2, z, z') \int_0^{r_2} \mathrm{d}r_1 \; f(r_1, z, z')$$

$$\sim W_{a,b}(2cr) j_L(\omega r) W_{a',b'}(2c'r) \qquad \sim M_{a,b}(2cr) j_L(\omega r) M_{a',b'}(2c'r)$$

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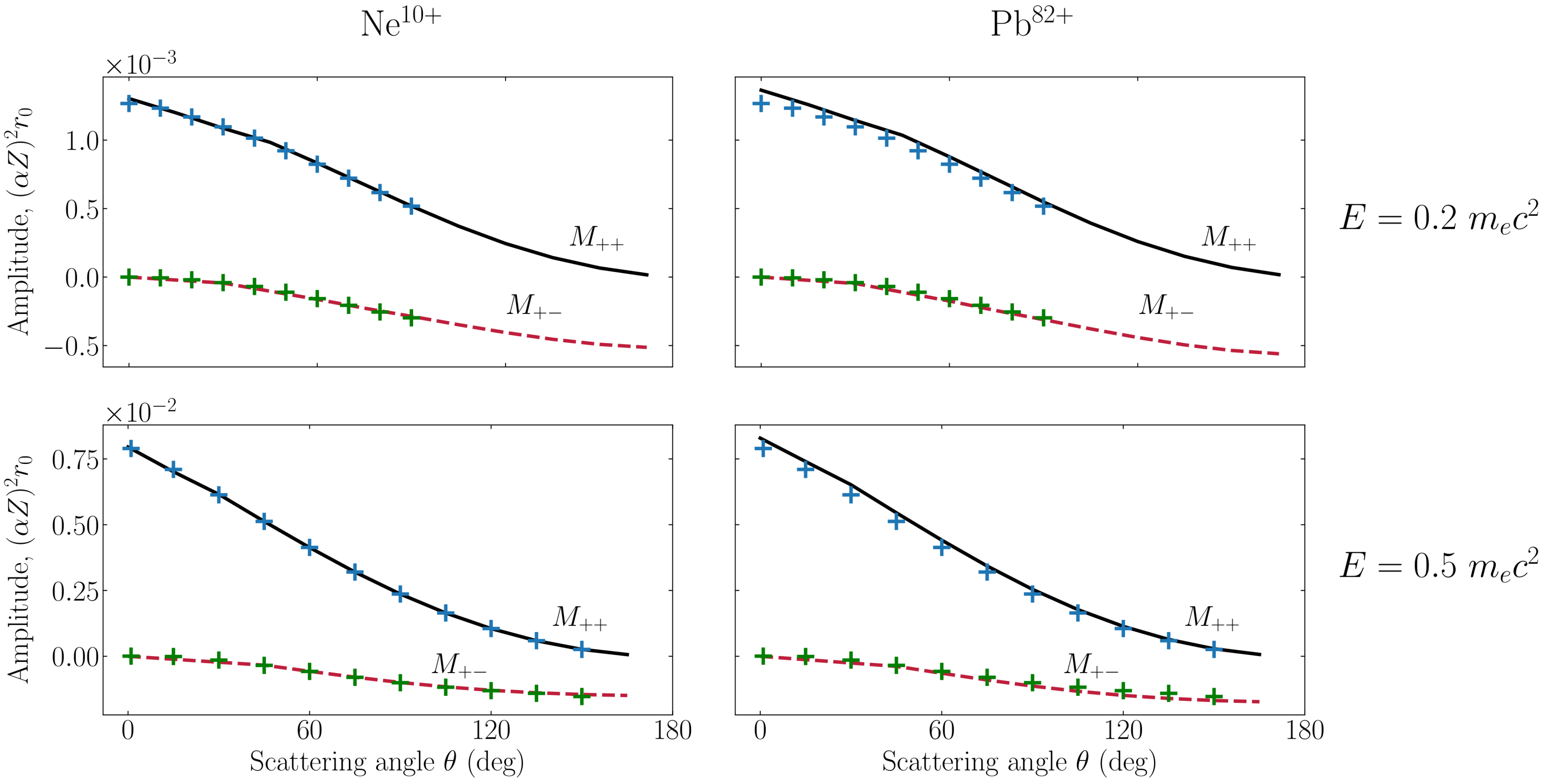
$$\sim W_{a,b}(2cr) j_L(\omega r) W_{a',b'}(2c'r) \qquad \sim M_{a,b}(2cr) j_L(\omega r) M_{a',b'}(2c'r)$$

We need $\sim 10^6$ of these integrals due to the many multipole combinations

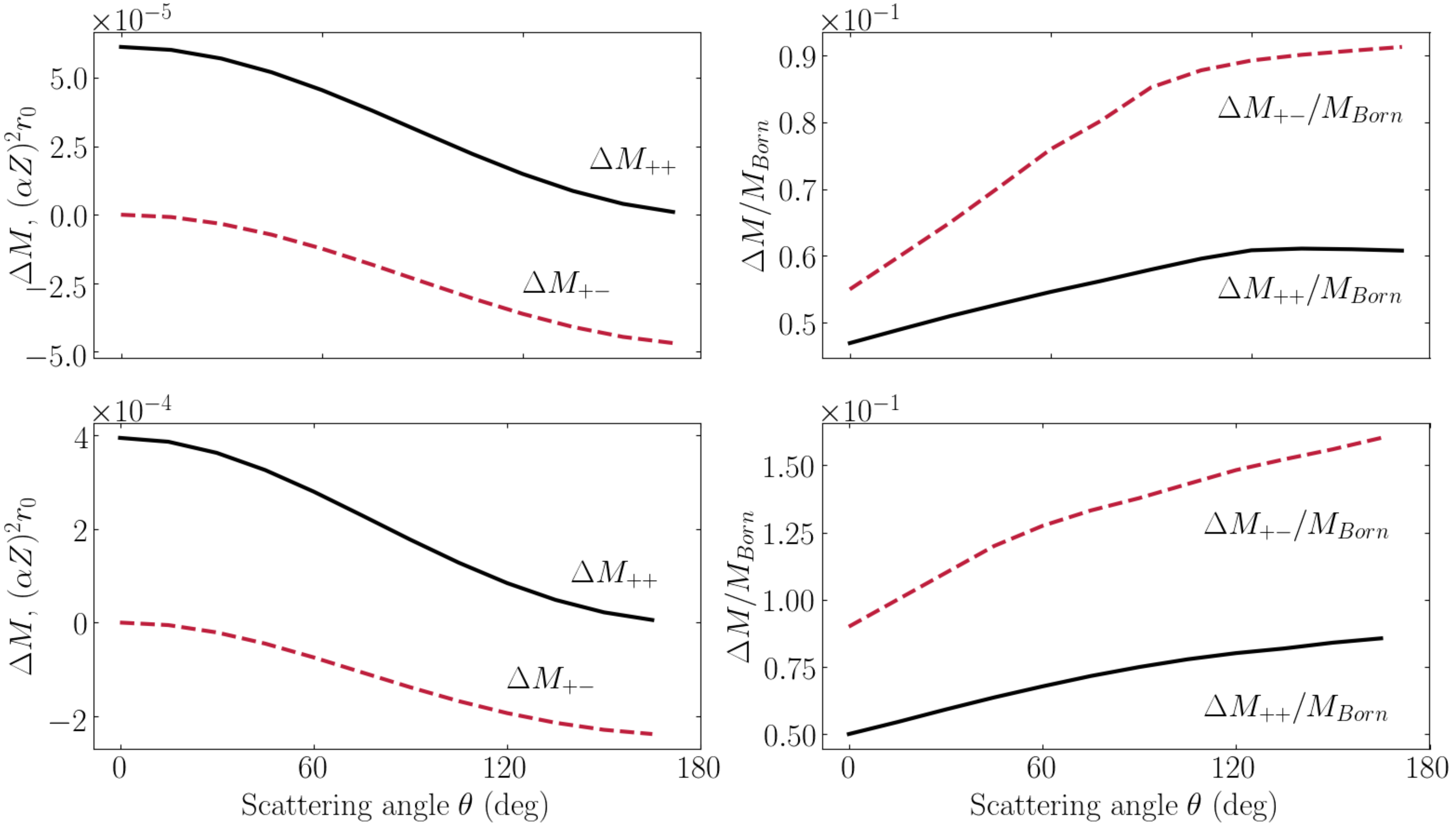
=> **Huge** computations

Delbrück Amplitude



Papatzacos and Mork, Phys. Rev. D 12, 206–218 (1975)
Falkenberg et al., Atomic Data and Nuclear Data Tables 50, 1–27 (1992)

Coulomb Corrections: Lead

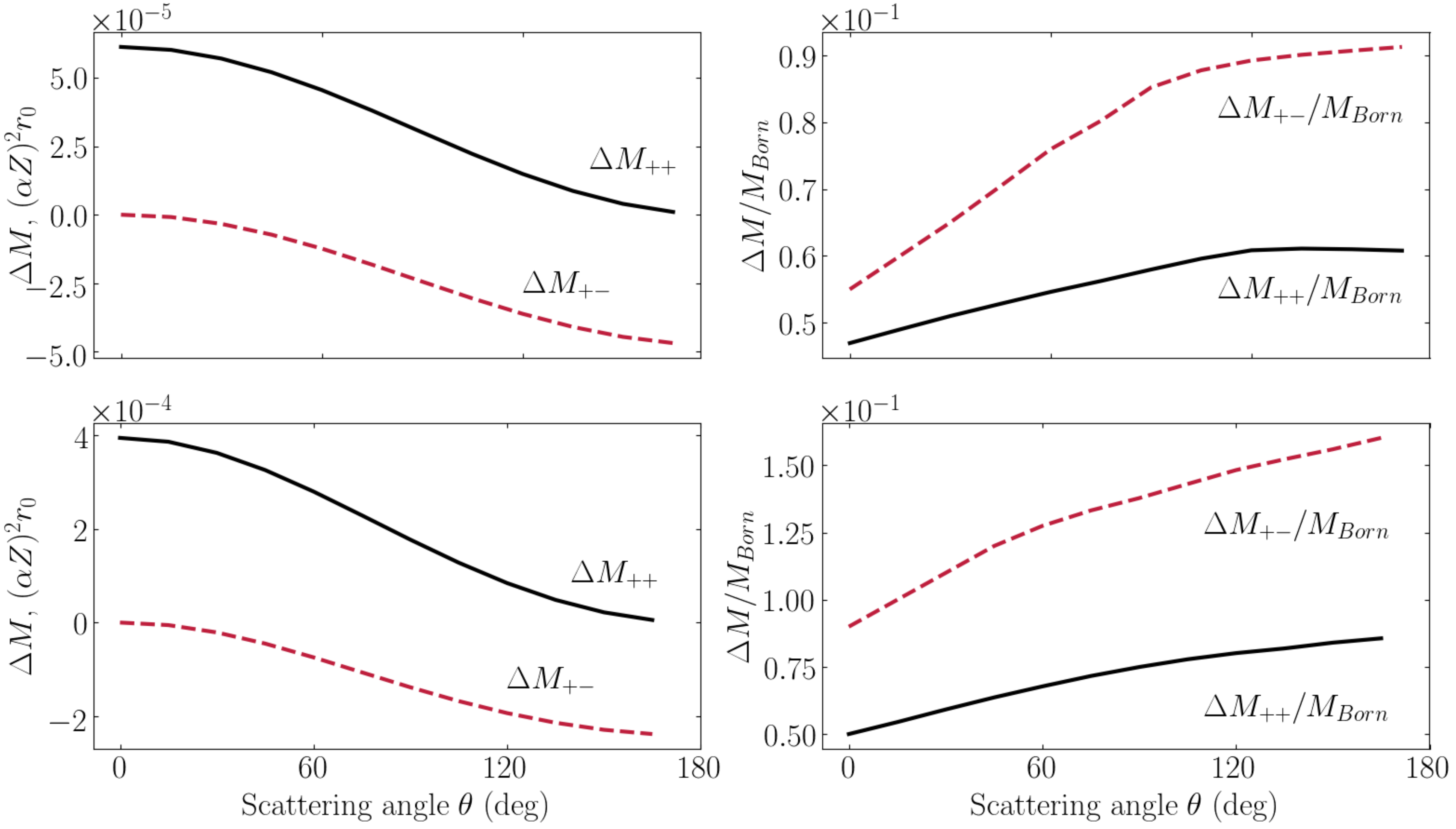


$E = 0.2\, m_e c^2$

$E = 0.5\, m_e c^2$

$$\Delta M_{\lambda_1 \lambda_2} = M_{\lambda_1 \lambda_2} - M_{\mathrm{Born}, \lambda_1 \lambda_2}$$

Coulomb Corrections: Lead



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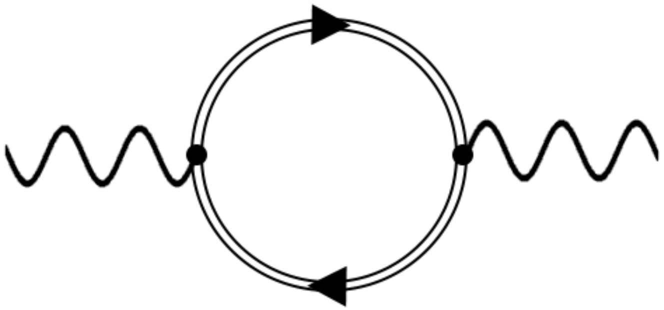
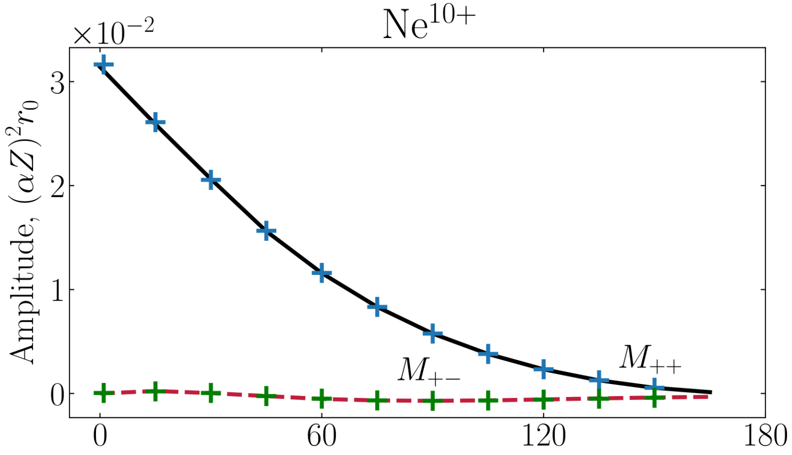
J. Sommerfeldt et al.,
Phys. Rev. A, 022804 (2022)

Summary

- New method to calculate Delbrück scattering which is exact (in αZ) has been developed

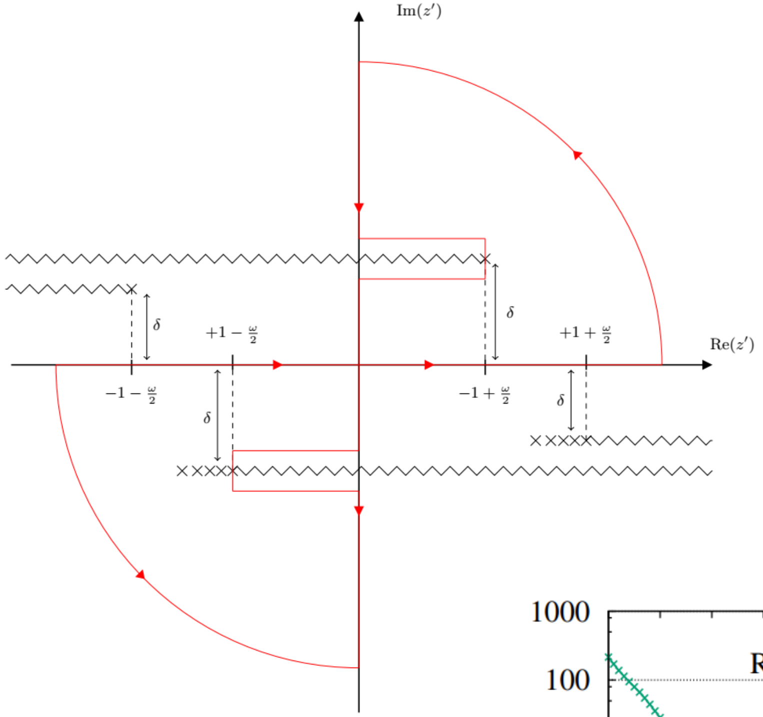


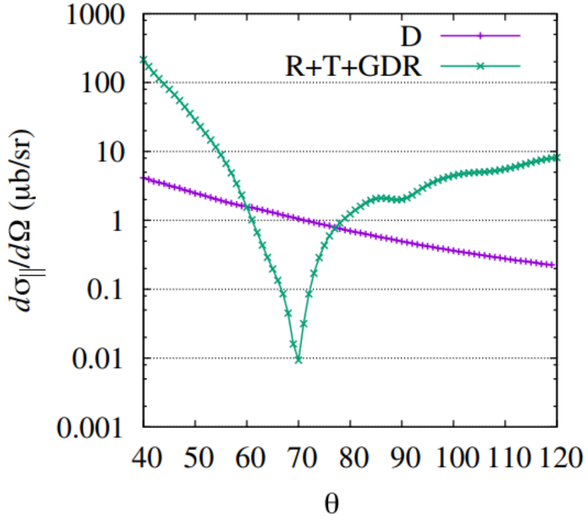
- It is possible to get accurate results in a reasonable computation time



Outlook

- There are a few adjustments needed to calculate amplitudes for above threshold energies
- Method can already be used to get high-accuracy predictions of Delbrück amplitudes





Koga and Hayakawa, PRL 118, 204801 (2017)

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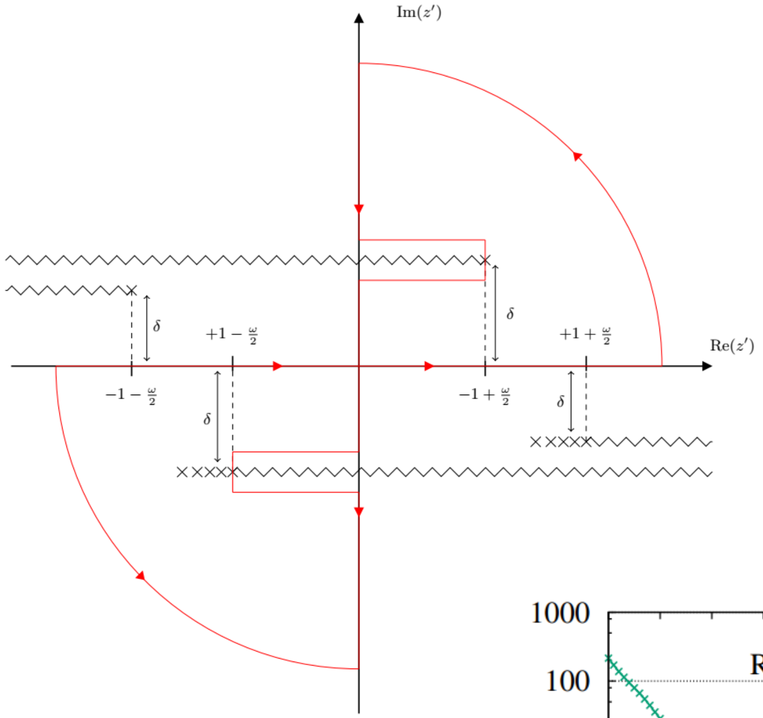
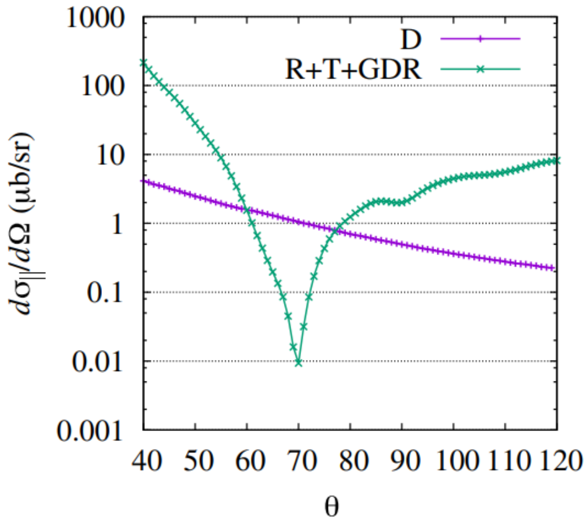


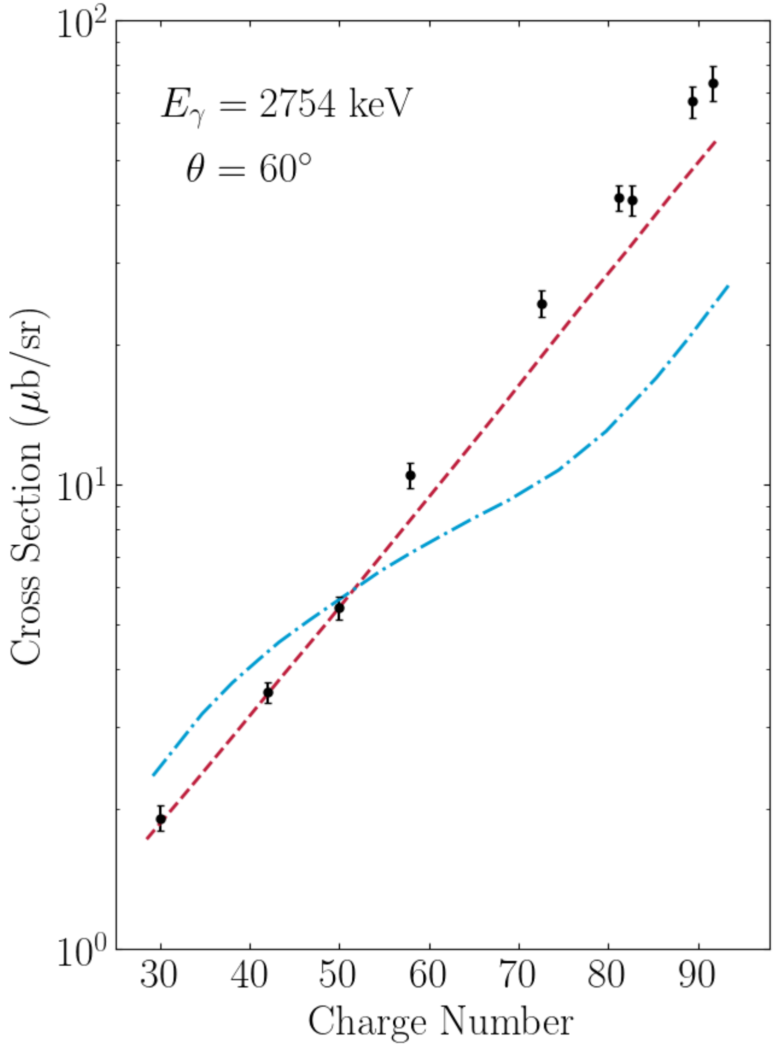
- Method can already be used to get high-accuracy predictions of Delbrück amplitudes

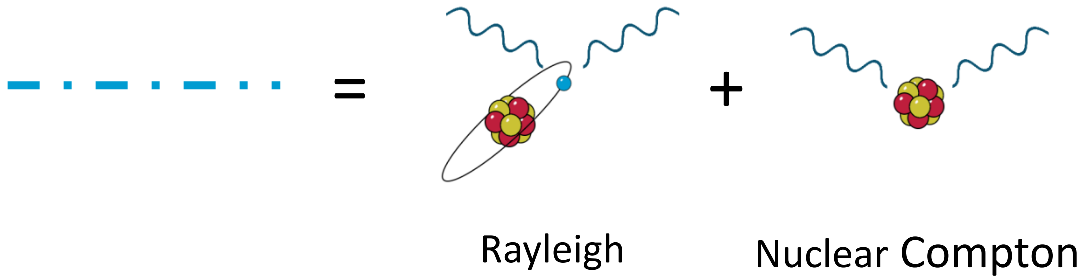


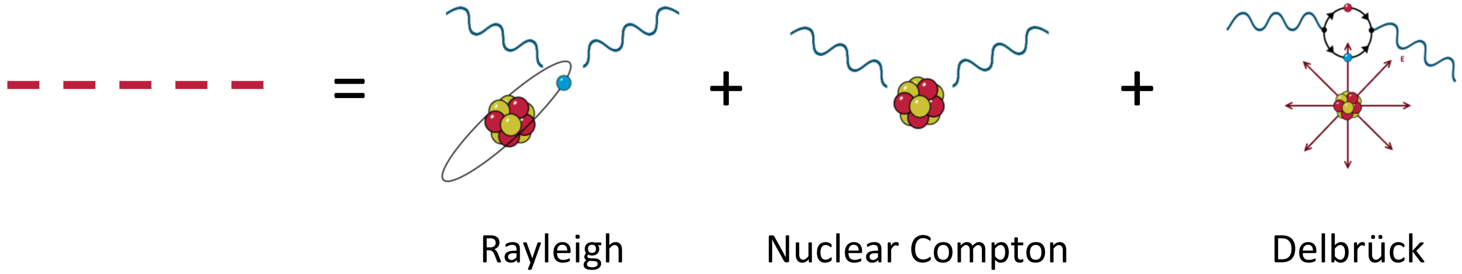
Koga and Hayakawa, PRL 118, 204801 (2017)

Collaborators: Vladimir Yerokhin, Robert Müller, Andrey Volotka, Vladimir Zaytsev, Andrey Surzhykov

Higher-Order Corrections

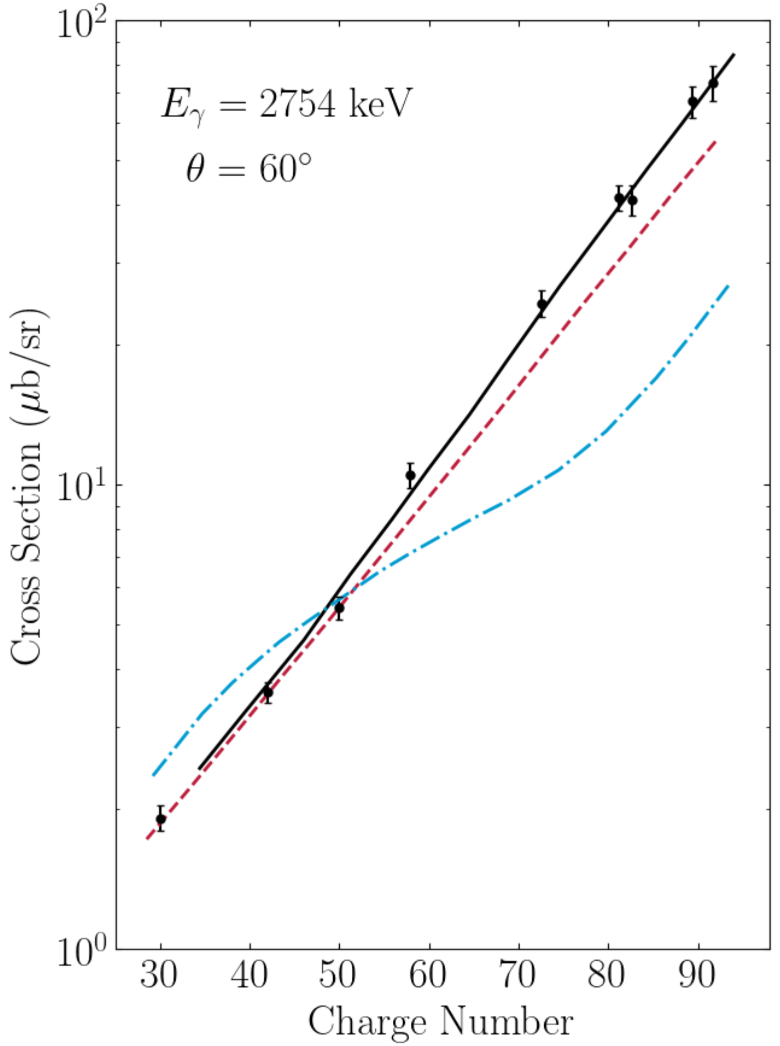


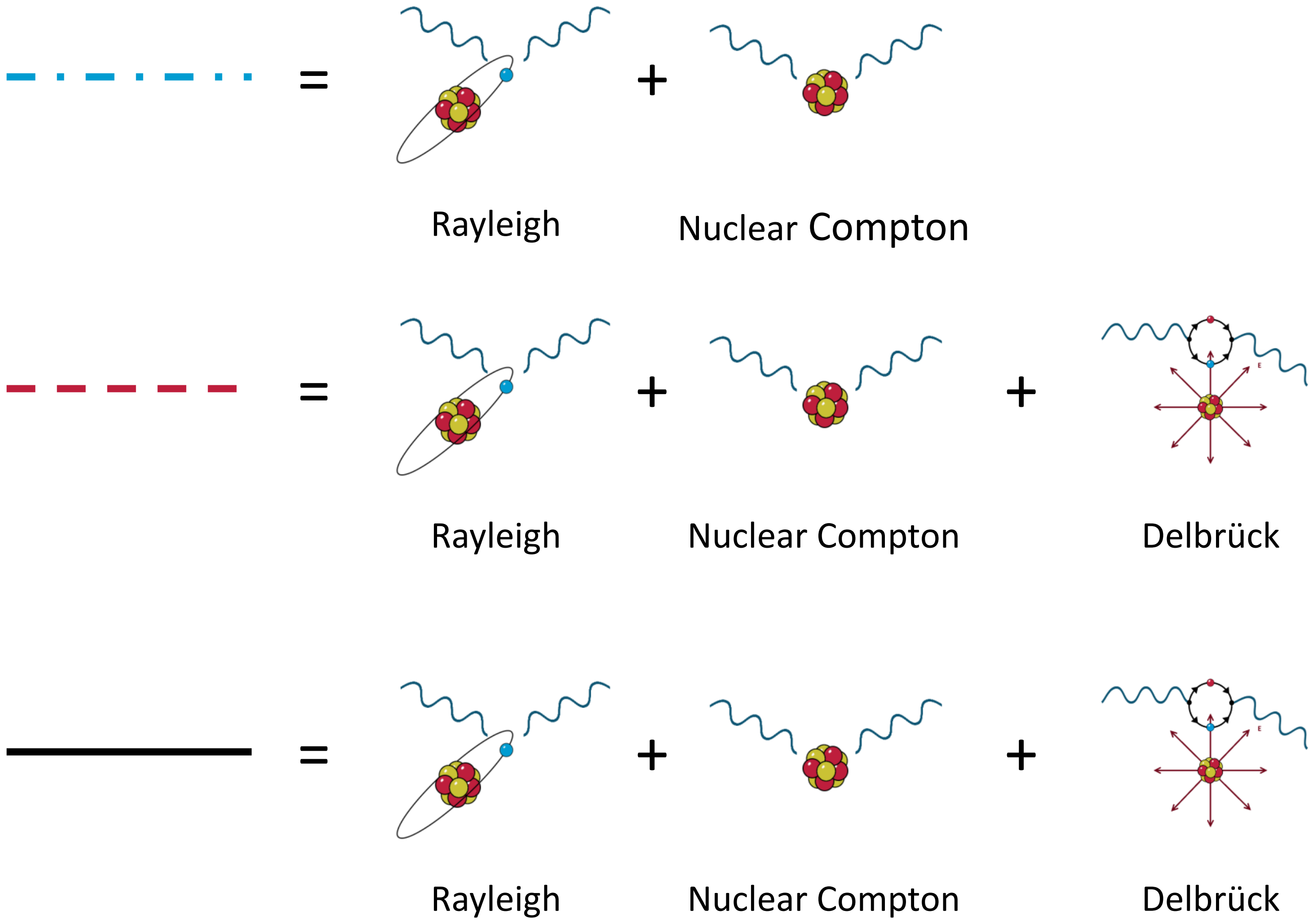




Kasten et al., Phys. Rev, C1606 (1986), pp. 1606-1615
Rullhusen et al., Phys. Rev, C23 (1981), pp. 1375-1383

Higher-Order Corrections





$+ \sim(\alpha Z)^4$

Kasten et al., Phys. Rev, C1606 (1986), pp. 1606-1615
Rullhusen et al., Phys. Rev, C23 (1981), pp. 1375-1383

Current Status of Delbrück Scattering Theory

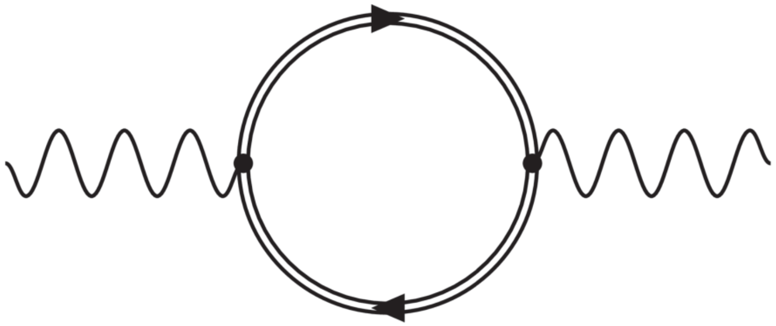
Almost all past theoretical studies were limited to some approximation:

- Lowest-order Born approximation
- High-energy small or large angle approximation
- Low-energy approximation

These approximations all fail for high nuclear charges, intermediate energies and arbitrary scattering angles!

$\Rightarrow$ No rigorous theoretical calculations were done that can be compared to the experimental data

$\Rightarrow$ Goal: Calculate full Feynman diagram with high numerical accuracy and stability



Radial Integral

The radial part of the integral is strongly oscillating and decreases only polynomially

$$K = \int_{-\infty}^{\infty} \mathrm{d}z' \int_{-\infty}^{\infty} \mathrm{d}z \, \delta(\omega + z - z') \boxed{\int_0^{\infty} \mathrm{d}r_2 \, g(r_2, z, z') \int_0^{r_2} \mathrm{d}r_1 \, f(r_1, z, z')}$$

=> First split the integral into parts that are close and and far away from the origin:

$$\boxed{\int_0^{\infty} \mathrm{d}r_2 \, g(r_2) \int_0^{r_2} \mathrm{d}r_1 \, f(r_1)} = \int_0^{a} \mathrm{d}r_2 \, g(r_2) \int_0^{r_2} \mathrm{d}r_1 \, f(r_1) + \int_a^{\infty} \mathrm{d}r_2 \, g(r_2) \int_0^{a} \mathrm{d}r_1 \, f(r_1)$$

$$+ \int_a^{\infty} \mathrm{d}r_2 \, g(r_2) \int_a^{r_2} \mathrm{d}r_1 \, f(r_1)$$

Radial Integral

Using **all** orders of the asymptotic expansion of the Whittaker functions

$$M_{\kappa,\mu}(x) \sim \frac{\Gamma(1+2\mu)}{\Gamma\left(\frac{1}{2}+\mu-\kappa\right)} \mathrm{e}^{\frac{1}{2}x} x^{-\kappa} \sum_{s=0}^{\infty} \frac{\left(\frac{1}{2}-\mu+\kappa\right)_s \left(\frac{1}{2}+\mu+\kappa\right)_s}{s!} x^{-s},$$

$$W_{\kappa,\mu}(z) \sim \mathrm{e}^{-\frac{1}{2}z} z^{\kappa} \sum_{s=0}^{\infty} \frac{\left(\frac{1}{2}+\mu-\kappa\right)_s \left(\frac{1}{2}-\mu-\kappa\right)_s}{s!} (-z)^{-s}$$

we can solve the integrals with large radial coordinates **analytically**:

$$\int_0^\infty \mathrm{d}r_2\, g(r_2) \int_0^{r_2} \mathrm{d}r_1\, f(r_1) = \underbrace{\boxed{\int_0^a \mathrm{d}r_2\, g(r_2) \int_0^{r_2} \mathrm{d}r_1\, f(r_1)}}_{\text{Numerical}} + \underbrace{\boxed{\int_a^\infty \mathrm{d}r_2\, g(r_2)}}_{\text{Analytical}} \underbrace{\boxed{\int_0^a \mathrm{d}r_1\, f(r_1)}}_{\text{Numerical}}$$

$$+ \underbrace{\boxed{\int_a^\infty \mathrm{d}r_2\, g(r_2) \int_a^{r_2} \mathrm{d}r_1\, f(r_1)}}_{\text{Analytical}}$$

First energy integral

We can solve the first energy integral trivially:

$$K = \int_{-\infty}^{\infty} \mathrm{d}z' \boxed{\int_{-\infty}^{\infty} \mathrm{d}z\ \delta(\omega + z - z')} \int_0^{\infty} \mathrm{d}r_2\ g(r_2, z, z') \int_0^{r_2} \mathrm{d}r_1\ f(r_1, z, z')$$

$$= \int_{-\infty}^{\infty} \mathrm{d}z' \ \int_0^{\infty} \mathrm{d}r_2\ g(r_2, z' - \omega, z') \int_0^{r_2} \mathrm{d}r_1\ f(r_1, z' - \omega, z')$$

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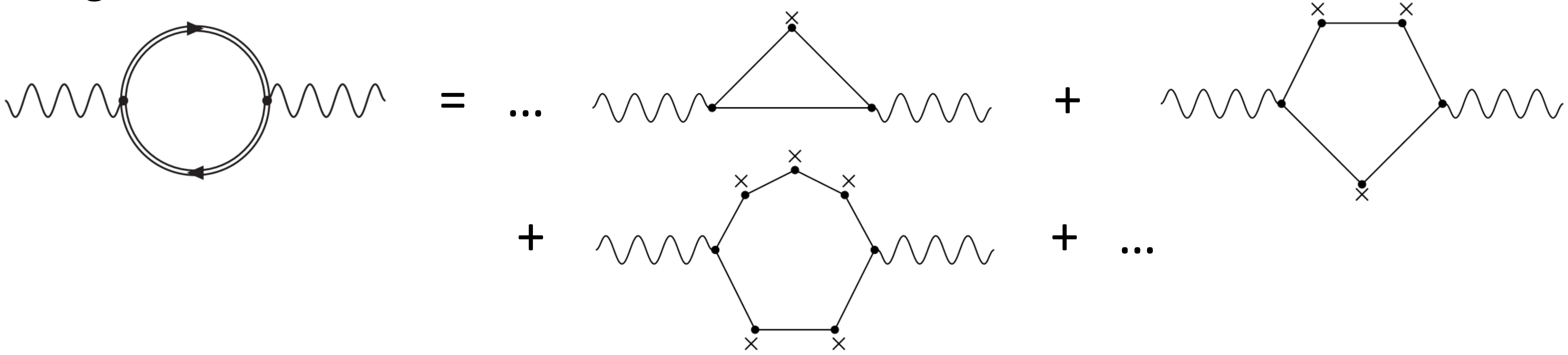
But then, terms proportional to odd powers of (αZ) vanish only after integration over z':



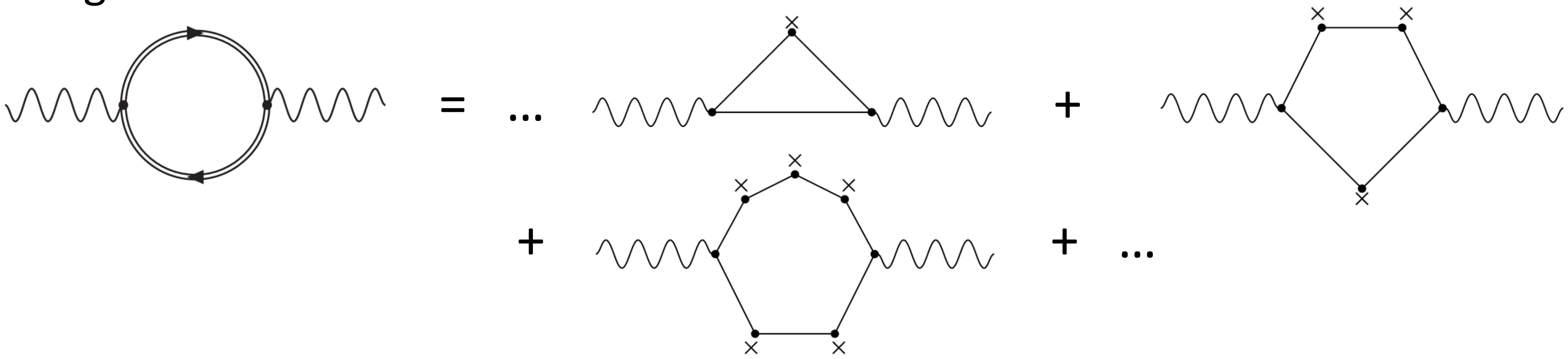
First energy integral

We instead choose a symmetric integrand for the first energy integral:

$$K = \int_{-\infty}^{\infty} \mathrm{d}z' \boxed{\int_{-\infty}^{\infty} \mathrm{d}z \; \delta(\omega + z - z')} \int_0^{\infty} \mathrm{d}r_2 \; g(r_2, z, z') \int_0^{r_2} \mathrm{d}r_1 \; f(r_1, z, z')$$

$$= \int_{-\infty}^{\infty} \mathrm{d}z' \; \int_0^{\infty} \mathrm{d}r_2 \; g(r_2, z' - \omega, z') \int_0^{r_2} \mathrm{d}r_1 \; f(r_1, z' - \omega, z')$$

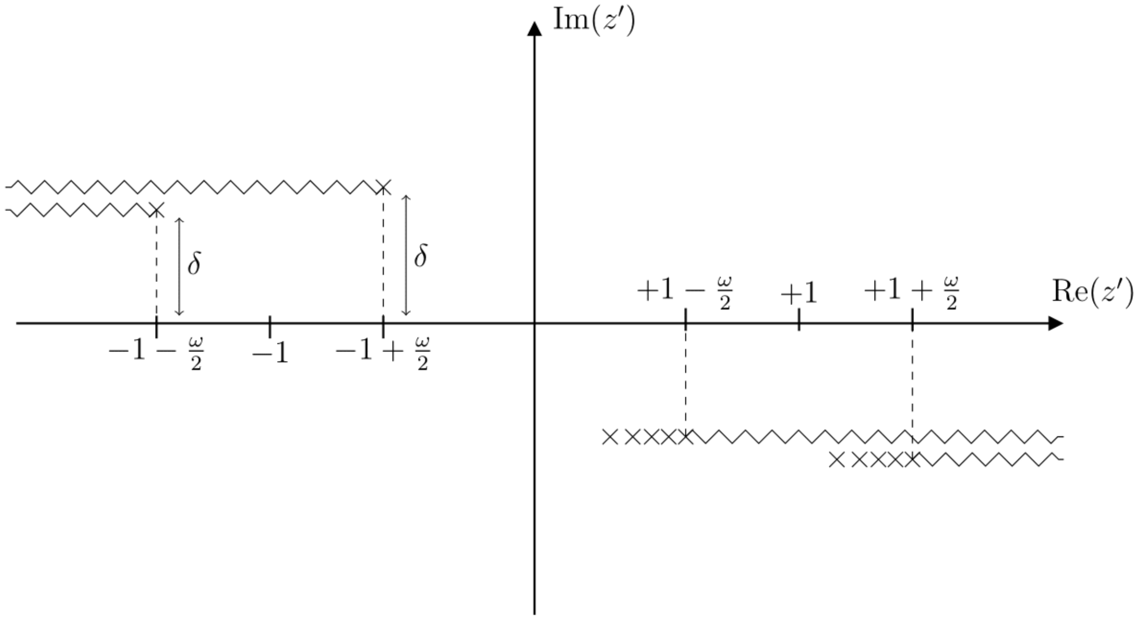
Now the integrand is symmetric to charge conjugation $Z \rightarrow -Z$ before the z' integration and the odd terms vanish



Second Energy integral

We are left with the integral over z'

$$K = \int_{-\infty}^{\infty} \mathrm{d}z' \ \int_0^{\infty} \mathrm{d}r_2 \ g(r_2, z' - \tfrac{\omega}{2}, z' + \tfrac{\omega}{2}) \int_0^{r_2} \mathrm{d}r_1 \ f(r_1, z' - \tfrac{\omega}{2}, z' + \tfrac{\omega}{2})$$



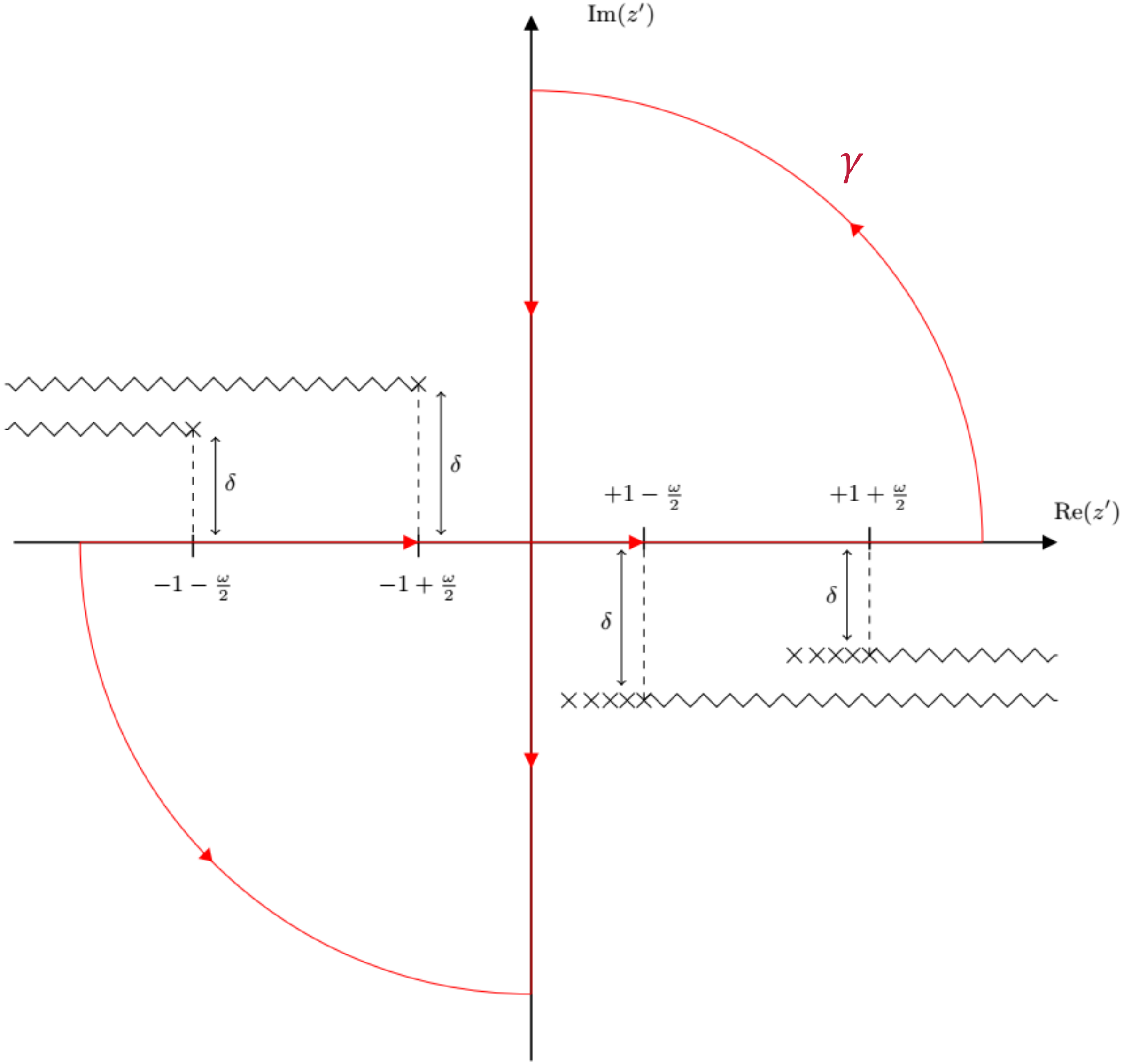
=> Integration along real axis is problematic due to the poles

Second Energy integral

We can turn the integration path to the imaginary axis by using the residue theorem:

$$\oint_\gamma f(z')\,\mathrm{d}z' = \boxed{2\pi i \sum_k \mathrm{Res}(f, a_k)}$$

= 0, since no poles are enclosed



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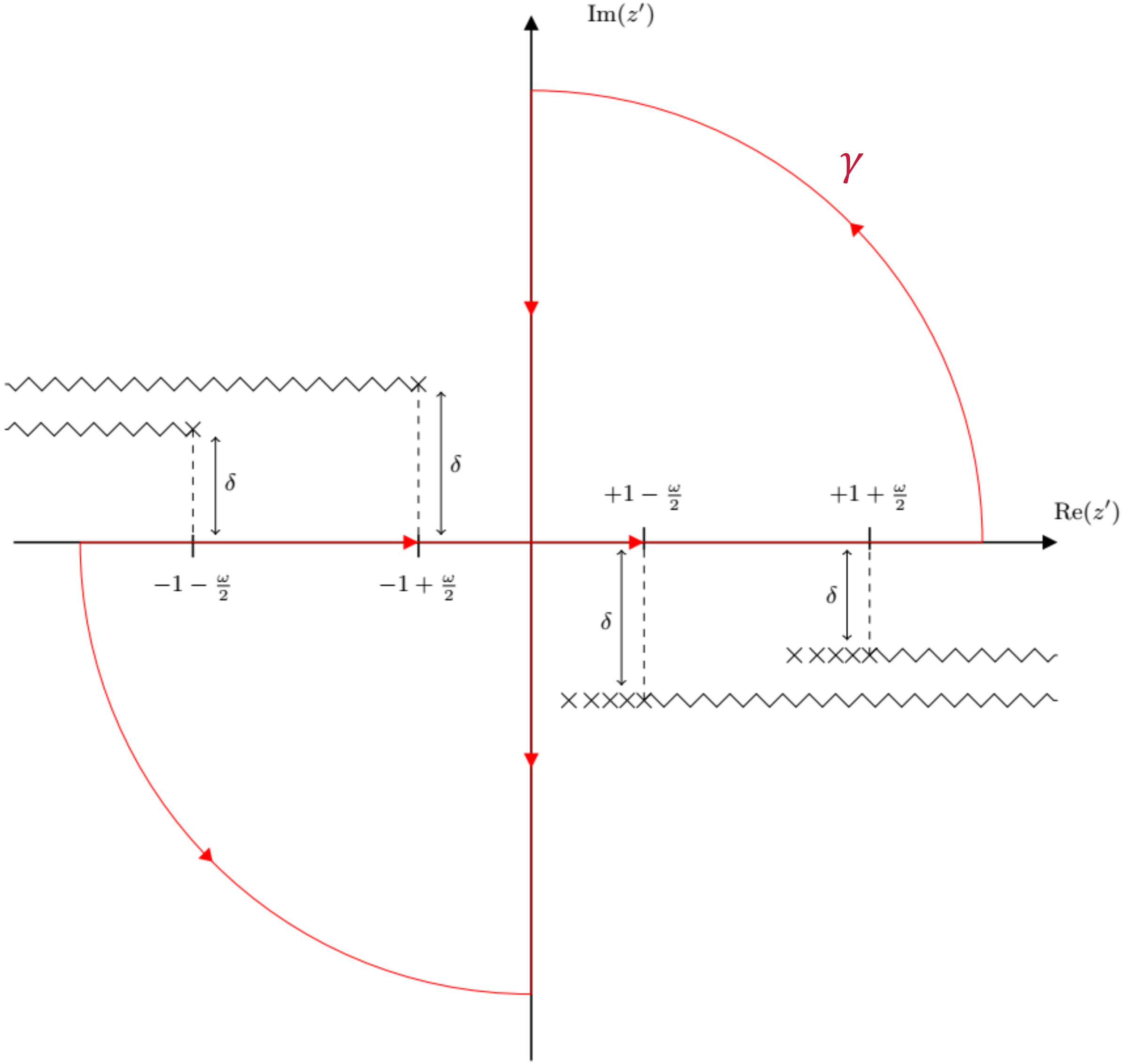
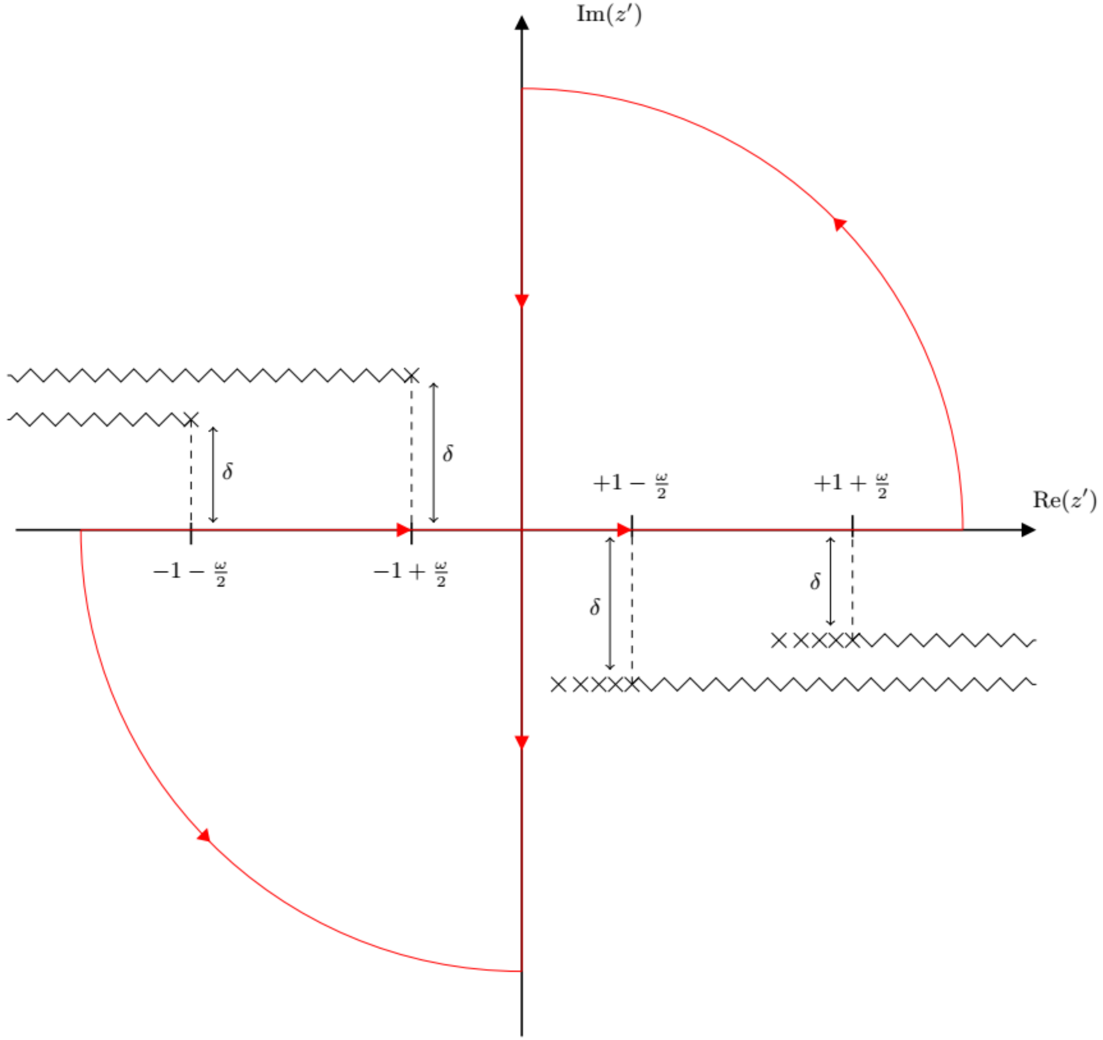


Unfortunately, the energy integral is divergent

Next objective: Above Threshold Calculations



For low energies, we saw that we can simply turn the integration path to the imaginary axis

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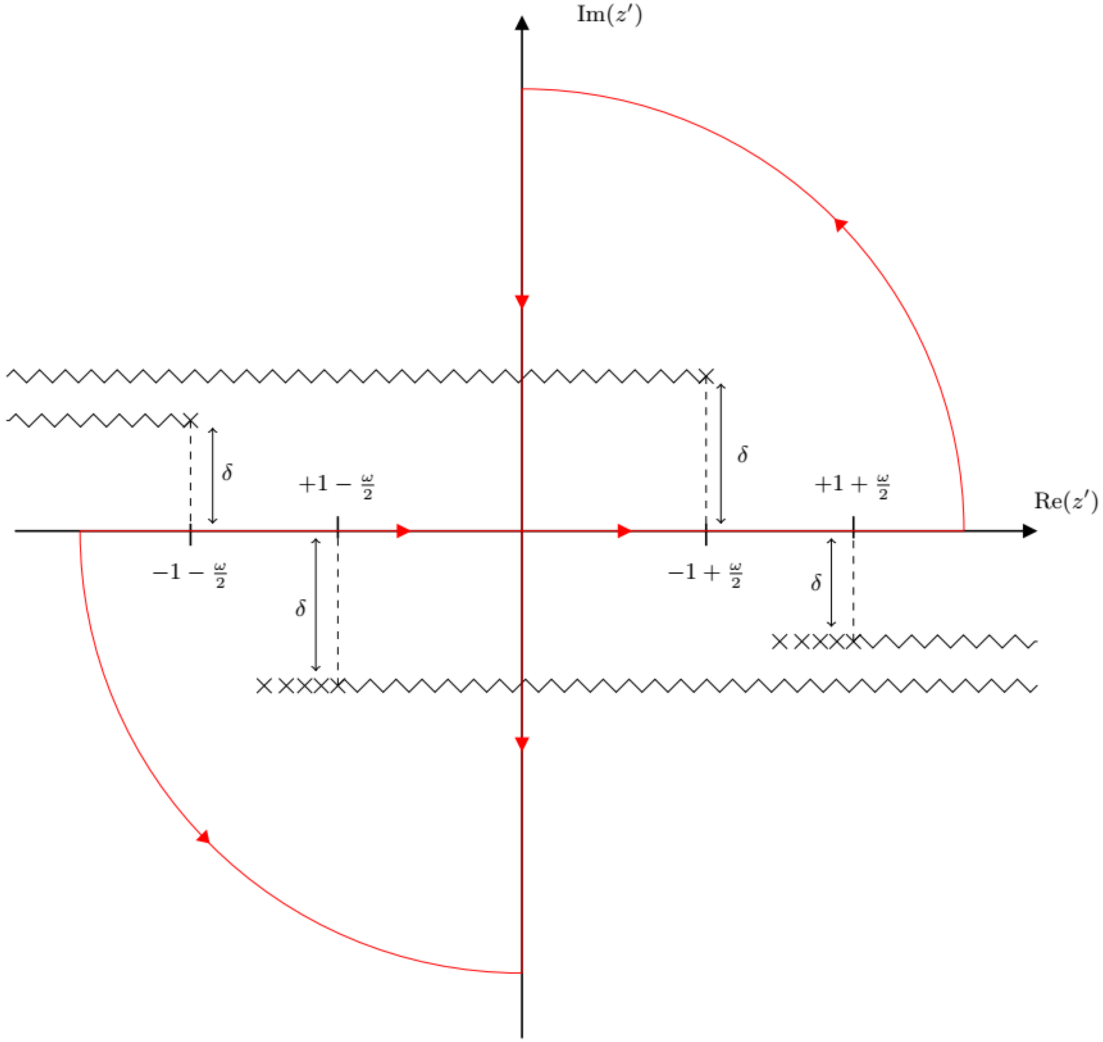
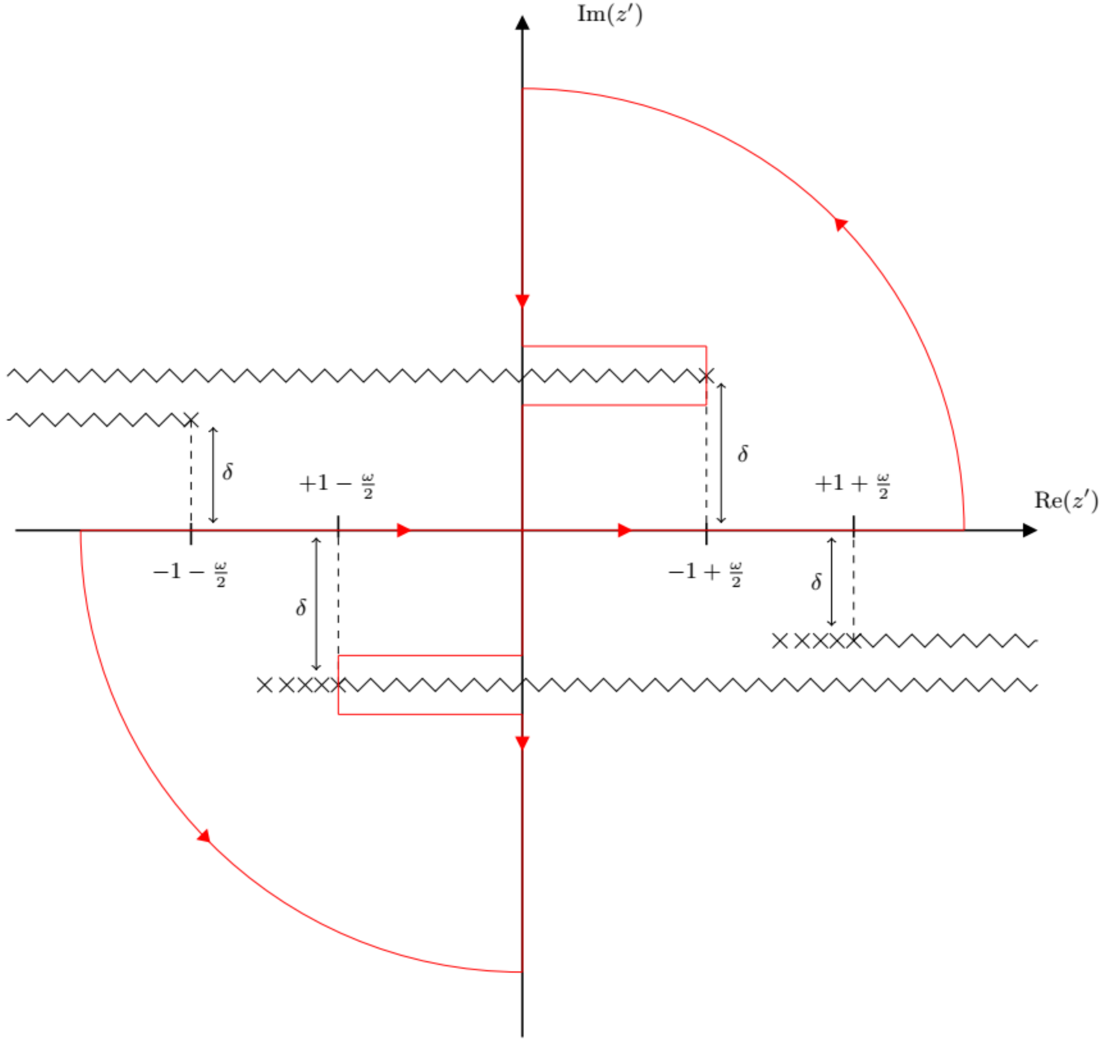


For low energies, we saw that we can simply turn the integration path to the imaginary axis

But for high energies above the pair production threshold, the branch cuts cross the imaginary axis

Next objective: Above Threshold Calculations

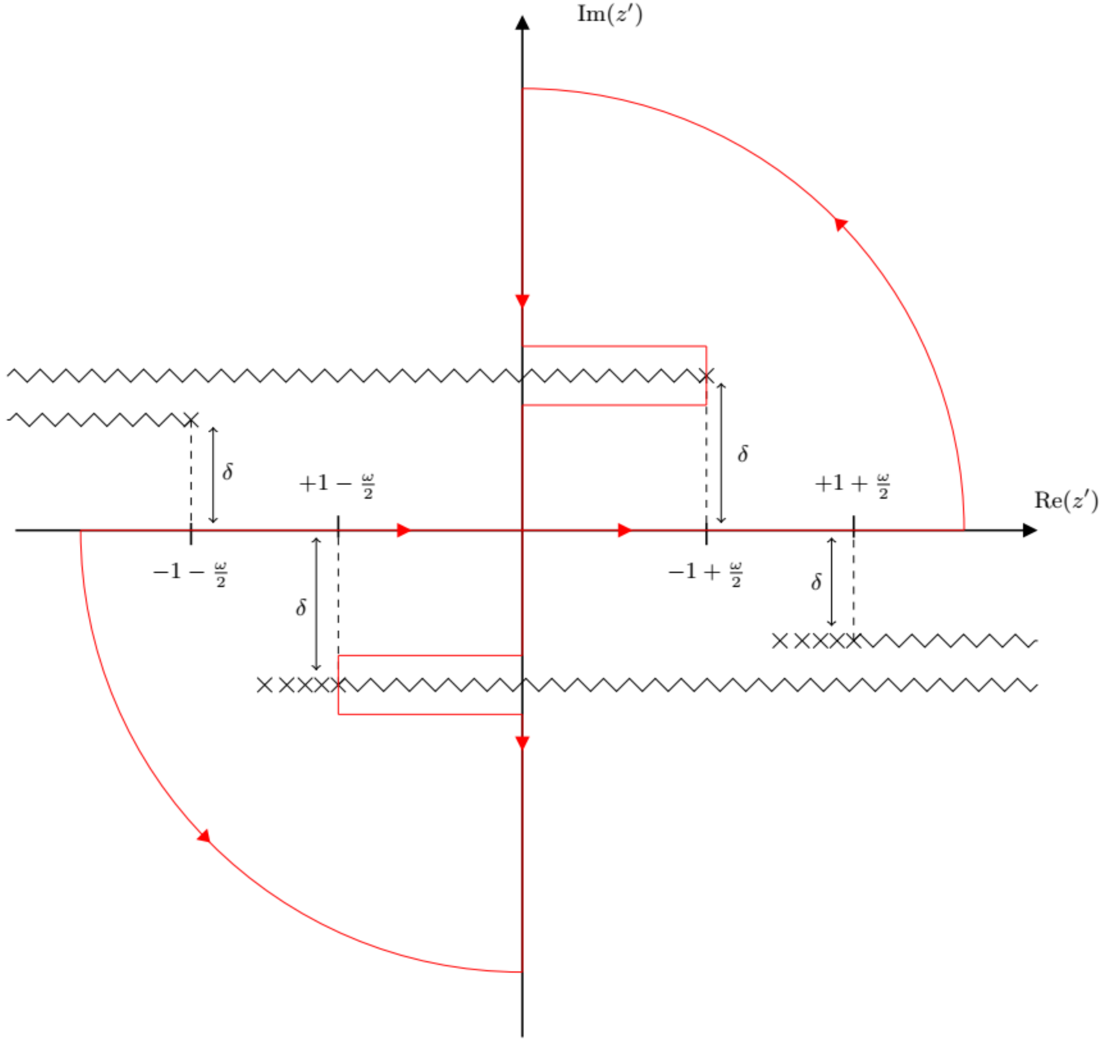


For low energies, we saw that we can simply turn the integration path to the imaginary axis

But for high energies above the pair production threshold, the branch cuts cross the imaginary axis

=> Integration path needs to be altered

Next objective: Above Threshold Calculations



For low energies, we saw that we can simply turn the integration path to the imaginary axis

But for high energies above the pair production threshold, the branch cuts cross the imaginary axis

=> Integration path needs to be altered

$$\oint_\gamma f(z')\,\mathrm{d}z' = \boxed{2\pi i \sum_k \mathrm{Res}(f, a_k)}$$

$\neq 0$, since the poles of the bound states are enclosed

Hybrid Parallelization on the PTB High-Perfomance Cluster

$$K = \int_{-\infty}^{\infty} \mathrm{d}z' \boxed{\int_0^{\infty} \mathrm{d}r_2 \; g(r_2, z' - \tfrac{\omega}{2}, z' + \tfrac{\omega}{2}) \int_0^{r_2} \mathrm{d}r_1 \; f(r_1, z' - \tfrac{\omega}{2}, z' + \tfrac{\omega}{2})}$$

MPI

Node 1

$$\int \mathrm{d}r_2 \; g(r_2, z_1 - \tfrac{\omega}{2}, z_1 + \tfrac{\omega}{2}) \int_0^{r_2} \mathrm{d}r_1 \; f(r_1, z_1 - \tfrac{\omega}{2}, z_1 + \tfrac{\omega}{2})$$

Evaluated in parallel using pthread

Node 2

$$\int \mathrm{d}r_2 \; g(r_2, z_2 - \tfrac{\omega}{2}, z_2 + \tfrac{\omega}{2}) \int_0^{r_2} \mathrm{d}r_1 \; f(r_1, z_2 - \tfrac{\omega}{2}, z_2 + \tfrac{\omega}{2})$$

Evaluated in parallel using pthread

...

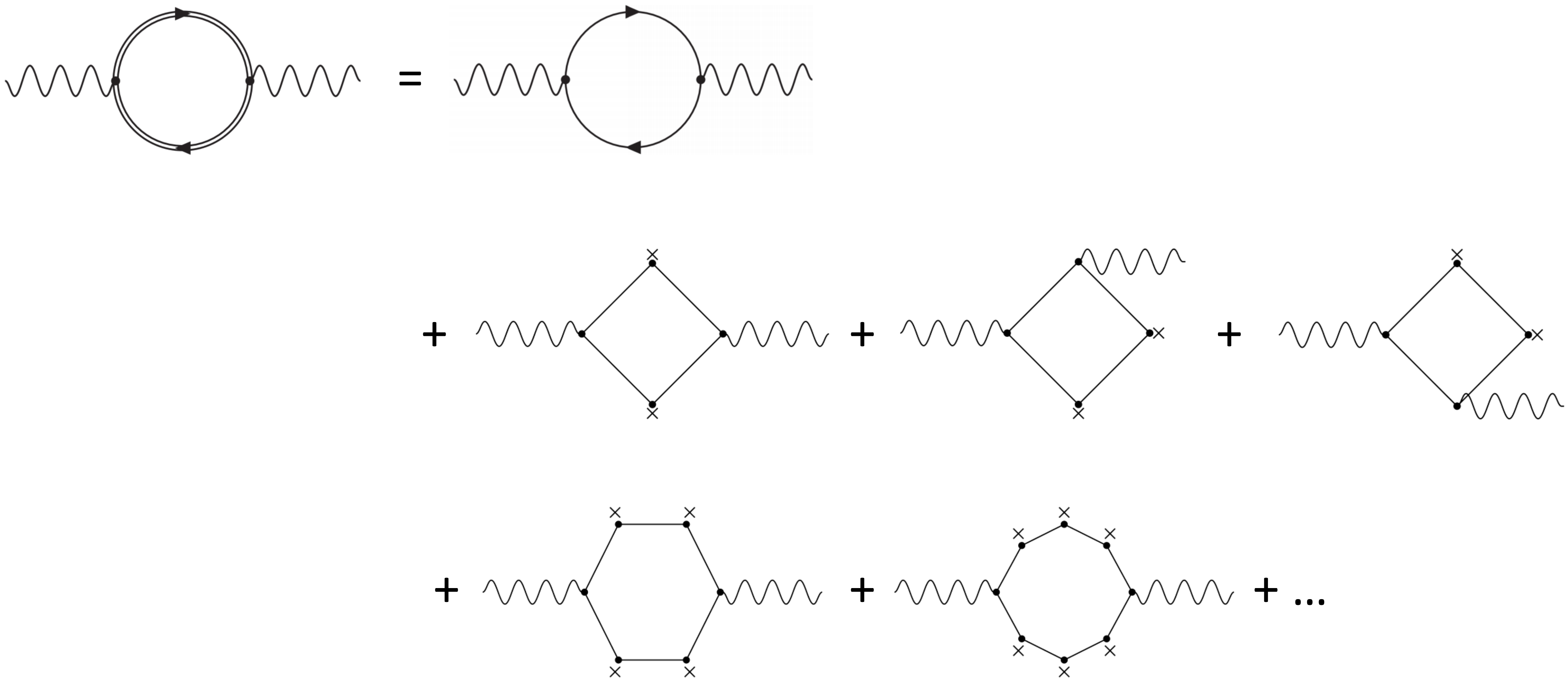
Node n

$$\int \mathrm{d}r_2 \; g(r_2, z_n - \tfrac{\omega}{2}, z_n + \tfrac{\omega}{2}) \int_0^{r_2} \mathrm{d}r_1 \; f(r_1, z_n - \tfrac{\omega}{2}, z_n + \tfrac{\omega}{2})$$

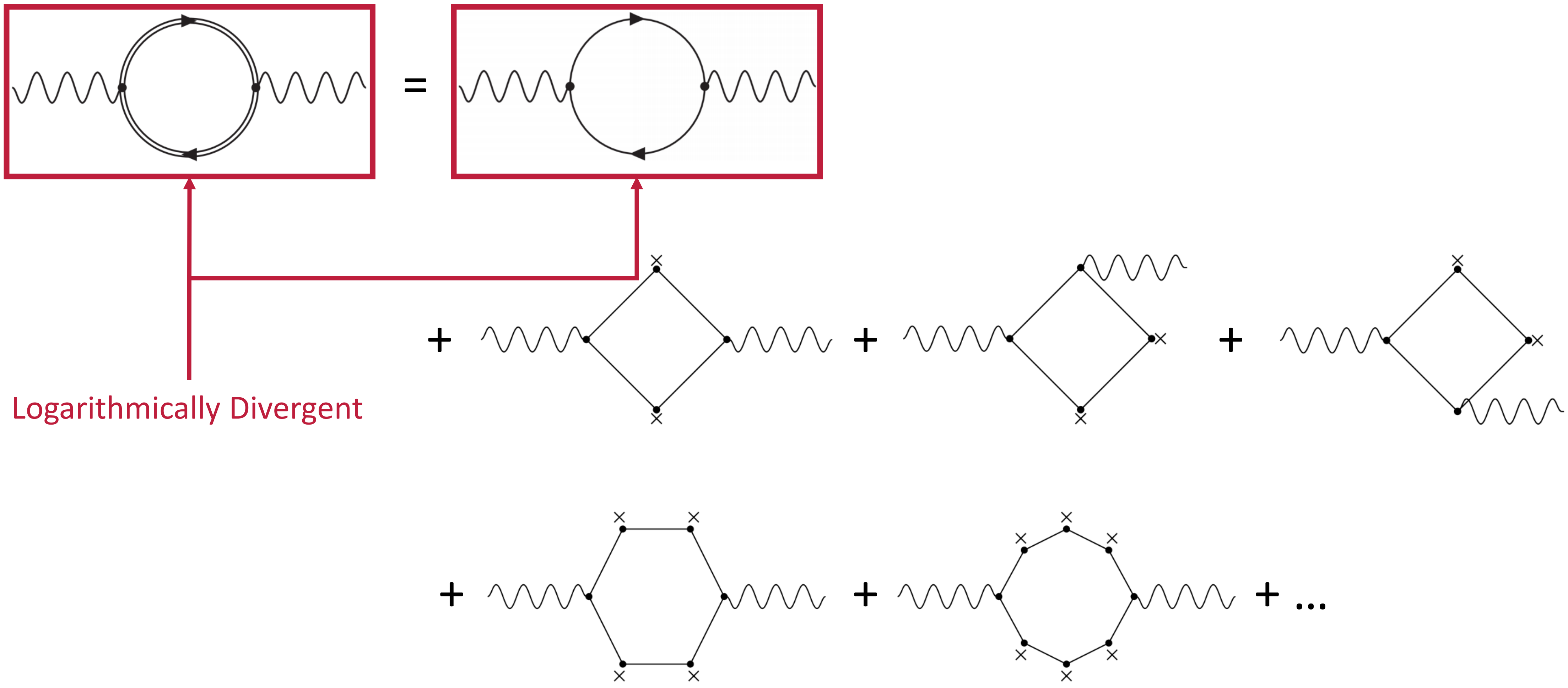
Evaluated in parallel using pthread

=> Computation times in the order of 1 day

Divergence of the Energy Integral

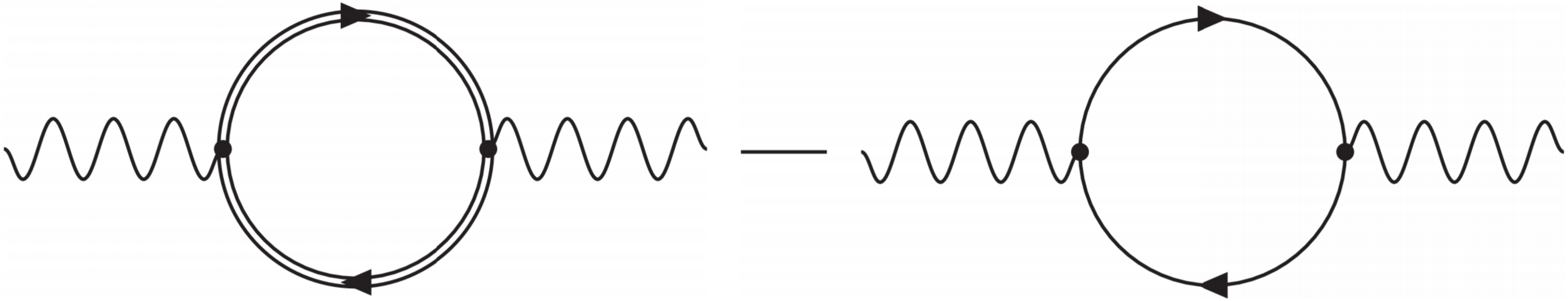


Divergence of the Energy Integral

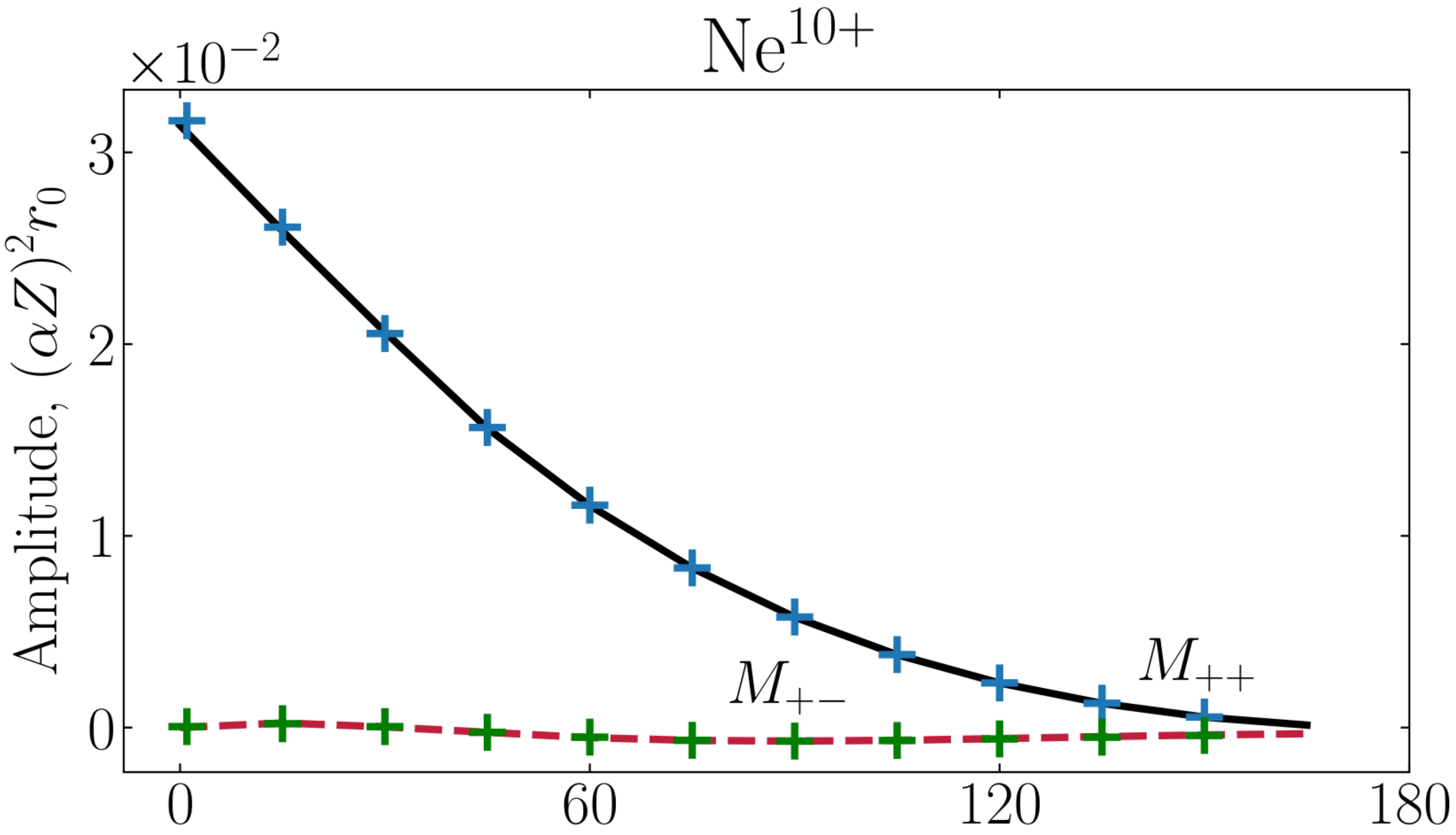


Divergence of the Energy Integral

Subtracting the free loop diagram cancels the divergence and we obtain a finite amplitude:



511 keV Calculation



Falkenberg et al., Atomic Data and Nuclear Data Tables 50, 1–27 (1992)

Delbrück Amplitude

We now know how to evaluate the function I, we just need to get convergence in the multipole expansions:

$$M = \sum_{\kappa\mu} \sum_{\kappa'\mu'} \sum_{P_1 L_1 M_1} \sum_{P_2 L_2 M_2} I(\omega, Z, P_1, L_1, M_1, P_2, L_2, M_2, \kappa, \mu, \kappa', \mu', \hat{k}_1, \hat{k}_2)$$

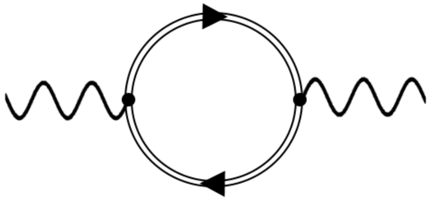
Delbrück Amplitude

We now know how to evaluate the function I, we just need to get convergence in the multipole expansions:

$$M = \boxed{\sum_{\kappa\mu}\sum_{\kappa'\mu'}}\boxed{\sum_{P_1L_1M_1}\sum_{P_2L_2M_2}} I(\omega, Z, P_1, L_1, M_1, P_2, L_2, M_2, \kappa, \mu, \kappa', \mu', \hat{k}_1, \hat{k}_2)$$

Slowly converging

Finite due to CG properties



$$\langle \kappa'\mu' | [\boldsymbol{Y}_{L_1} \otimes \boldsymbol{\sigma}]_{L_1M_1} | -\kappa\mu \rangle \langle \kappa'\mu' | [\boldsymbol{Y}_{L_2} \otimes \boldsymbol{\sigma}]_{L_2M_2} | -\kappa\mu \rangle^*$$

Sum over κ and κ‘

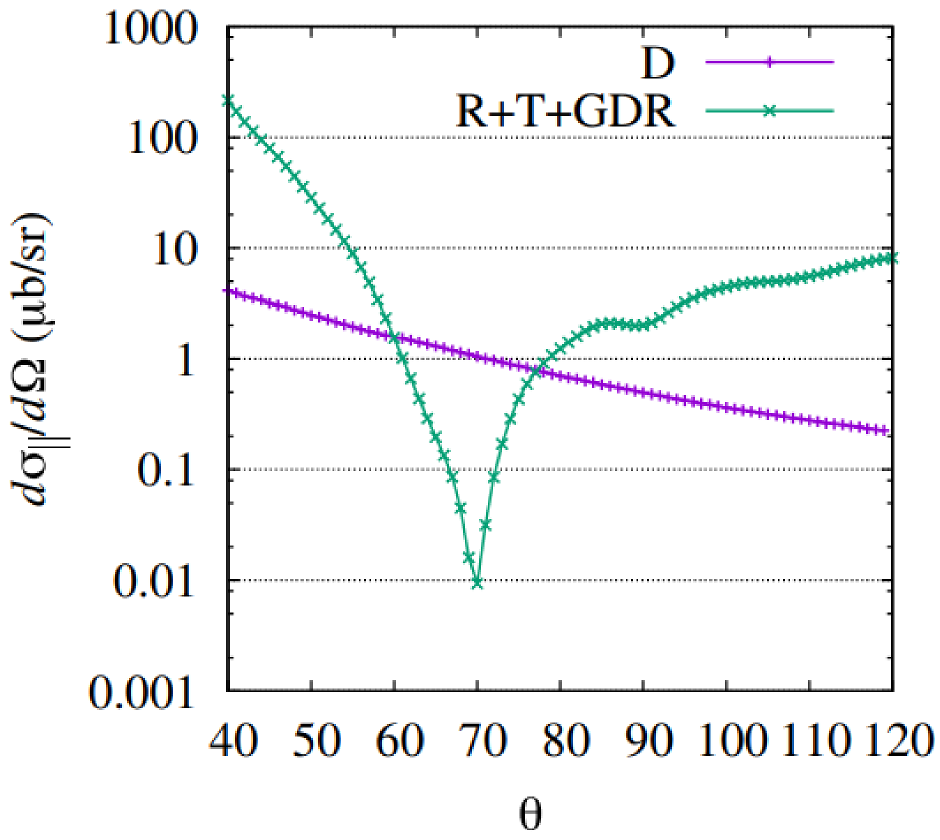
To improve the convergence, we rewrite the sum over κ and κ’ as the sum over one single parameter *j*

$$M = \sum_{\kappa,\kappa'} X_{\kappa\kappa'} = \sum_{|\kappa|,|\kappa'|} \sum_{sign(\kappa)} \sum_{sign(\kappa')} X_{\kappa\kappa'} = \sum_{|\kappa|,|\kappa'|} X_{|\kappa|,|\kappa'|} = \sum_{j} Y_j$$

Y_1	Y_2	Y_3	Y_4	Y_5
$X_{1,1}$	$X_{1,2}$	$X_{1,3}$	$X_{1,4}$	$X_{1,5}$
$X_{2,1}$	$X_{2,2}$	$X_{2,3}$	$X_{2,4}$	$X_{2,5}$
$X_{3,1}$	$X_{3,2}$	$X_{3,3}$	$X_{3,4}$	$X_{3,5}$
$X_{4,1}$	$X_{4,2}$	$X_{1,3}$	$X_{4,4}$	$X_{4,5}$
$X_{5,1}$	$X_{5,2}$	$X_{5,3}$	$X_{5,4}$	$X_{5,5}$

Least-squares inverse-polynomial fitting is used to estimate the tail of the expansion

Elastic Scattering of Polarized Photons



Koga and Hayakawa, PRL 118, 204801 (2017)

Even for energies as low as $\omega = 1100$ keV, Delbrück scattering of polarized photons is dominant for certain scattering angles

Problems with the integration

1. Poles of the integrand
2. Integral over r_2 decreases very slowly
3. Integral over r_1 increases exponentially
4. Many of these integrals have to be calculated

For example, for $L_{max} = \kappa_{max} = 30$, we need:

#Integrals = 30*30*60*60*4*128 = 1,658,880,000

$\Rightarrow$ Computation time using a naive implementation and Mathematicas hypergeometric functions:

~ $2.3*10^5$ years

Solution: Integral over r_1 increases exponentially

The Whittaker M function can be expressed as:

$$M_{\nu-\frac{1}{2},\lambda}(2cr) = e^{-cr}(2cr)^{\frac{1}{2}+\lambda}M(1+\lambda-\nu, 1+2\lambda, 2cr)$$

And after a Kummer transformation of the confluent hypergeometric function:

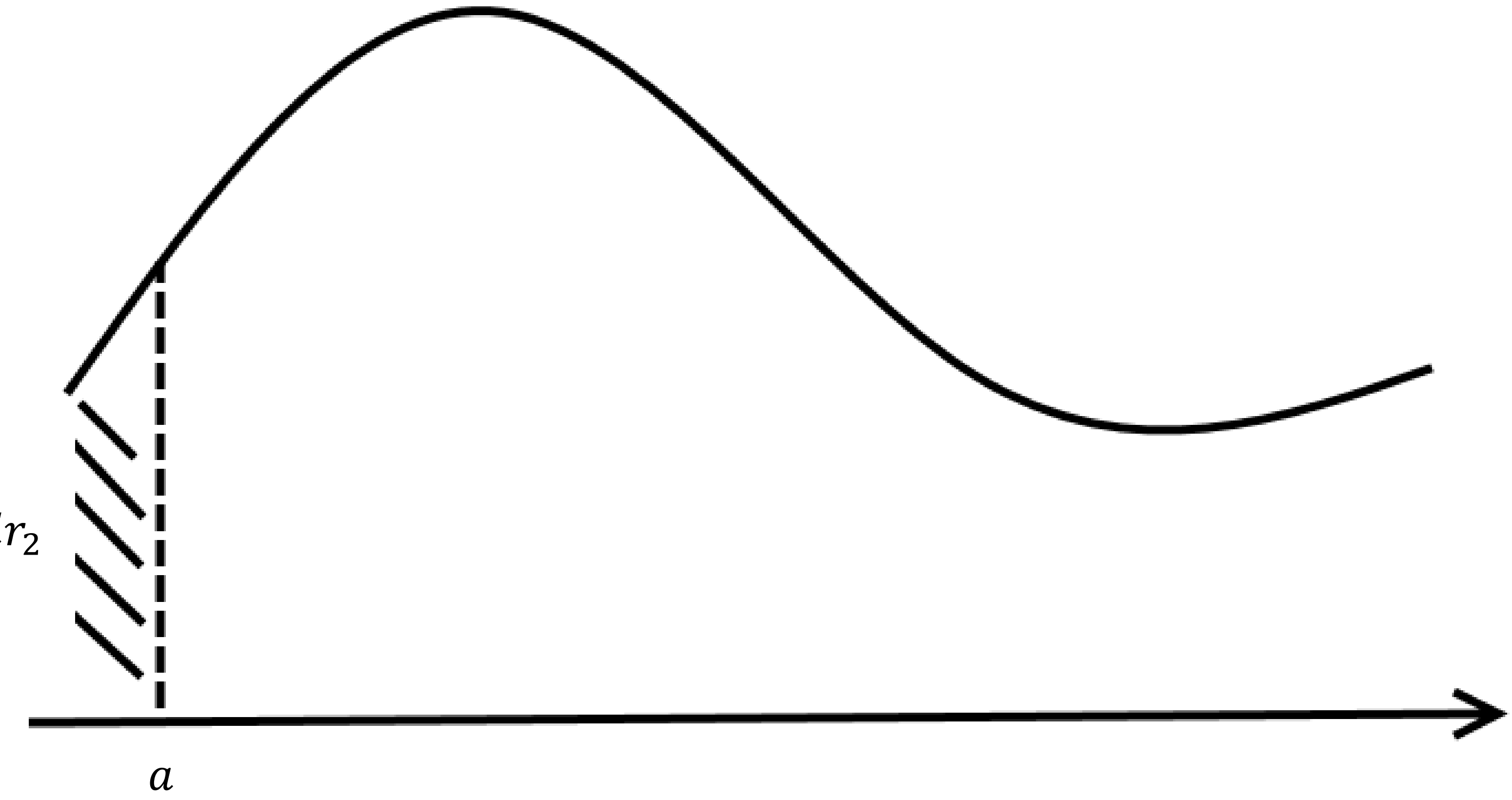
$$M_{\nu-\frac{1}{2},\lambda}(2cr) = e^{+cr}(2cr)^{\frac{1}{2}+\lambda}M(\lambda+\nu, 1+2\lambda, -2cr)$$

This exponential increase can be cancelled by:

$$W_{\nu-\frac{1}{2},\lambda}(2cr) = e^{-cr}(2cr)^{\frac{1}{2}+\lambda}U(1+\lambda-\nu, 1+2\lambda, 2cr)$$

Solution: Integral over r_1 increases exponentially

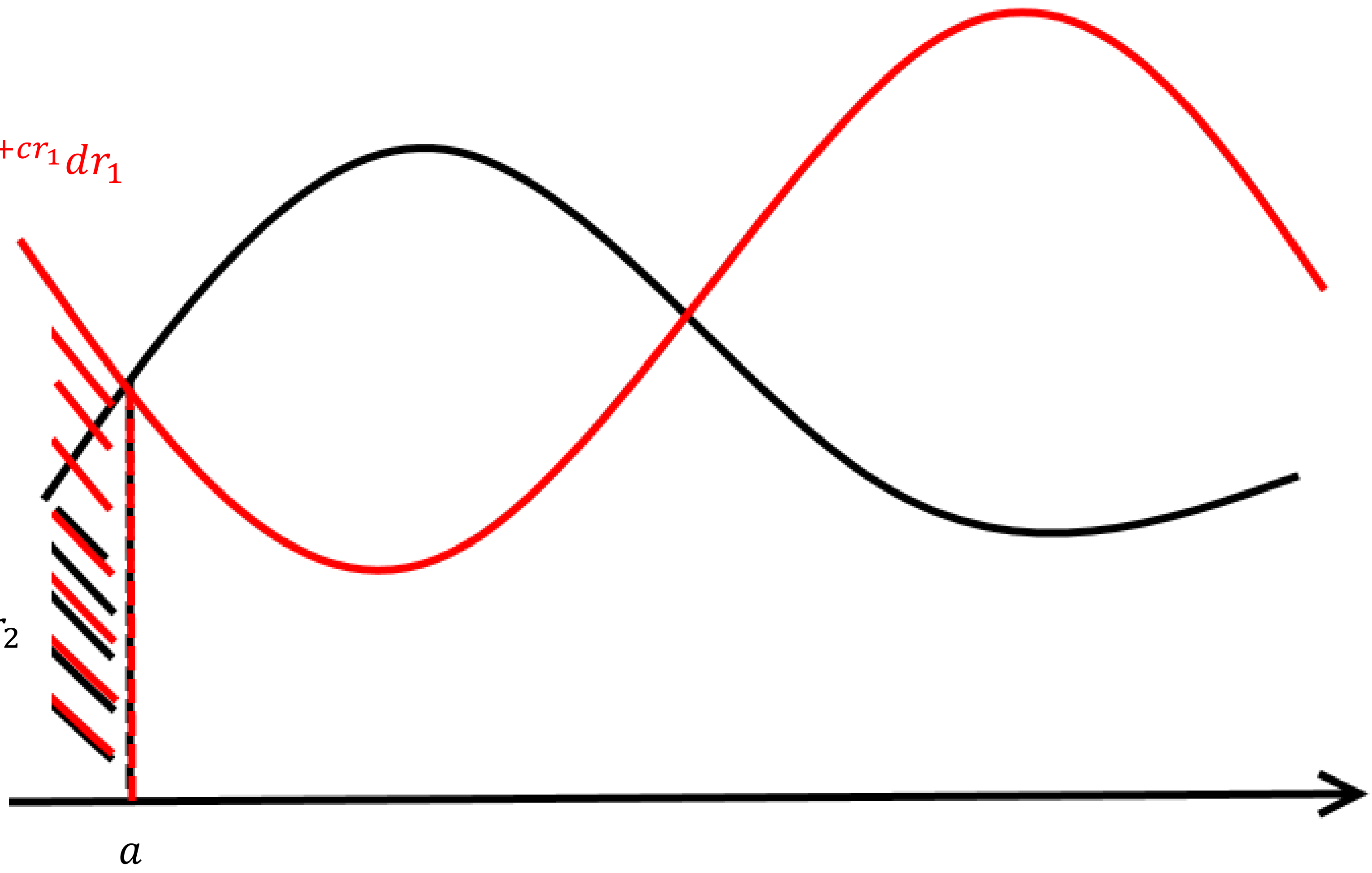
$$I_2(a) = \int_0^a \ldots e^{-cr_2} I_1(r_2) dr_2$$



Solution: Integral over r_1 increases exponentially

$$e^{-ca} I_1(a) = e^{-ca} \int_0^a \ldots e^{+cr_1} dr_1$$

$$I_2(a) = \int_0^a \ldots e^{-cr_2} I_1(r_2) dr_2$$



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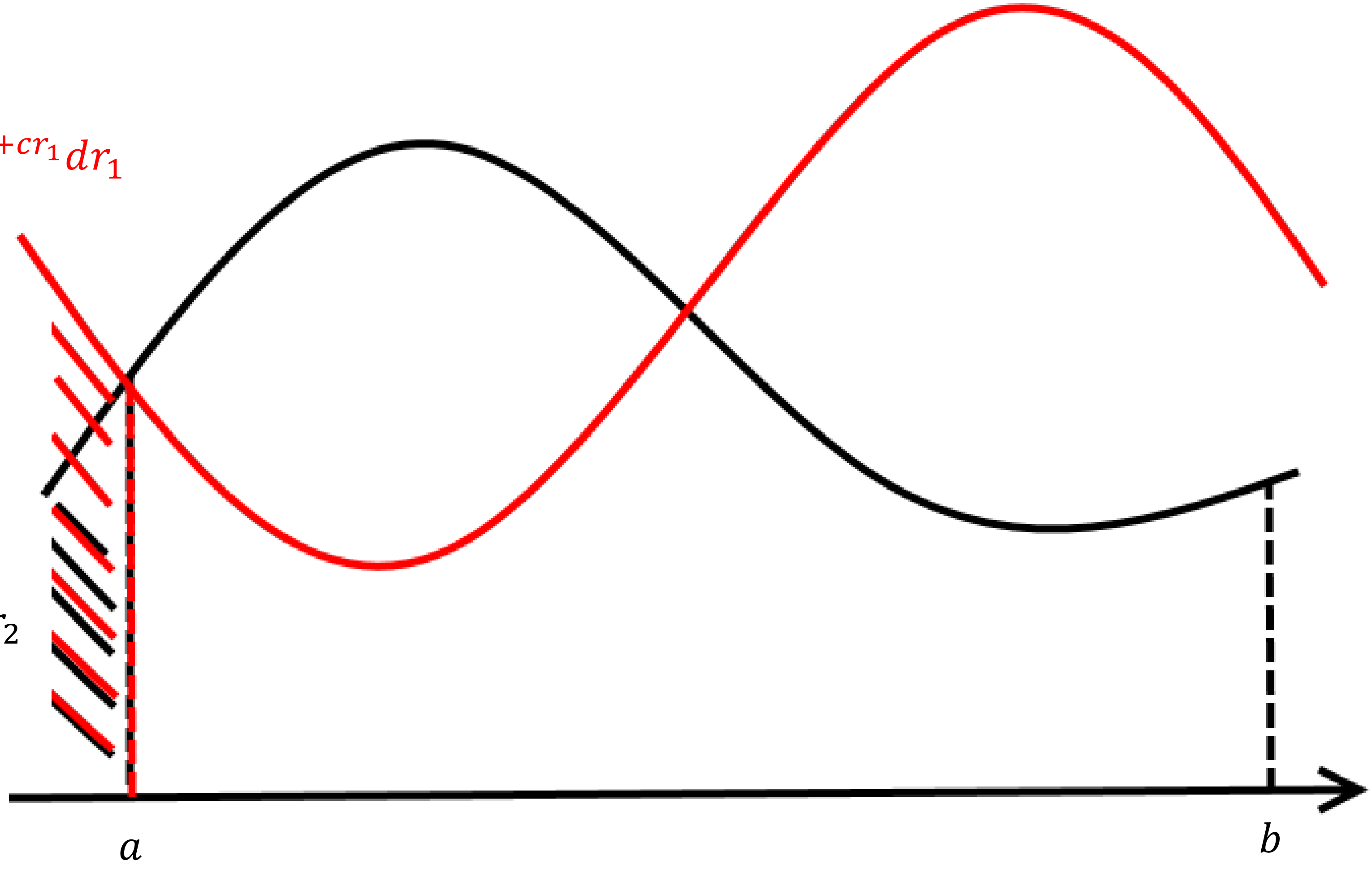

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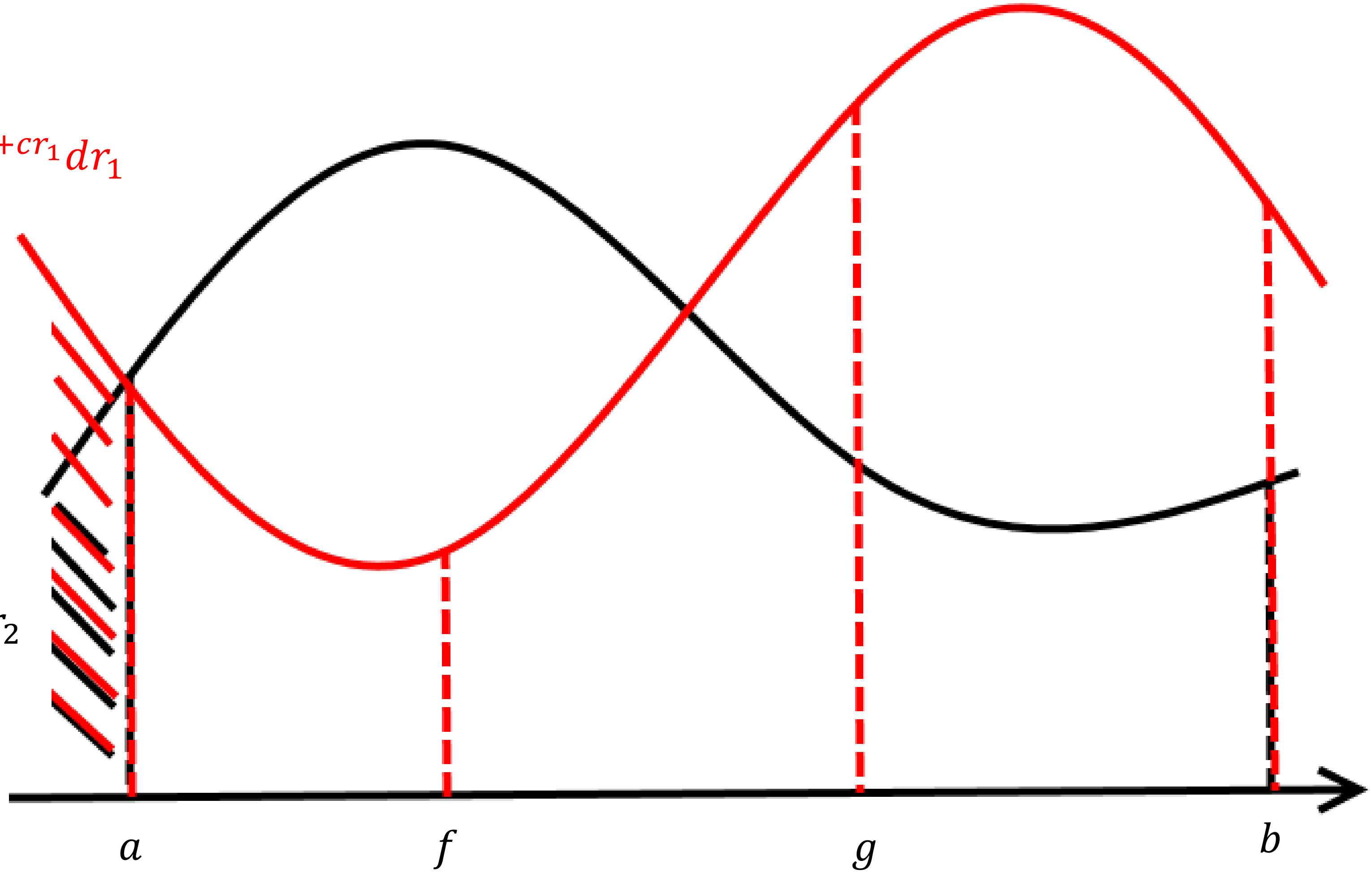

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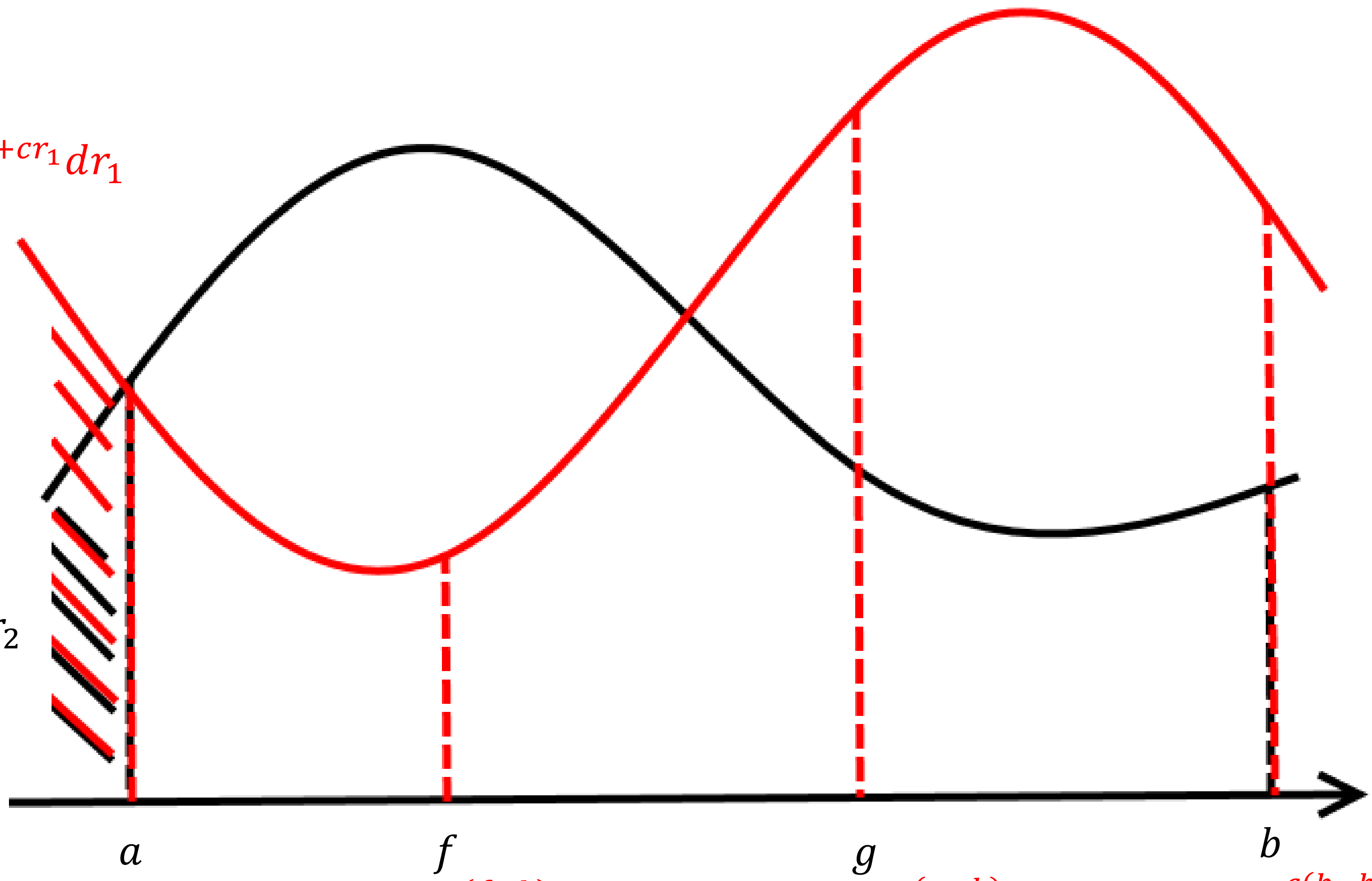
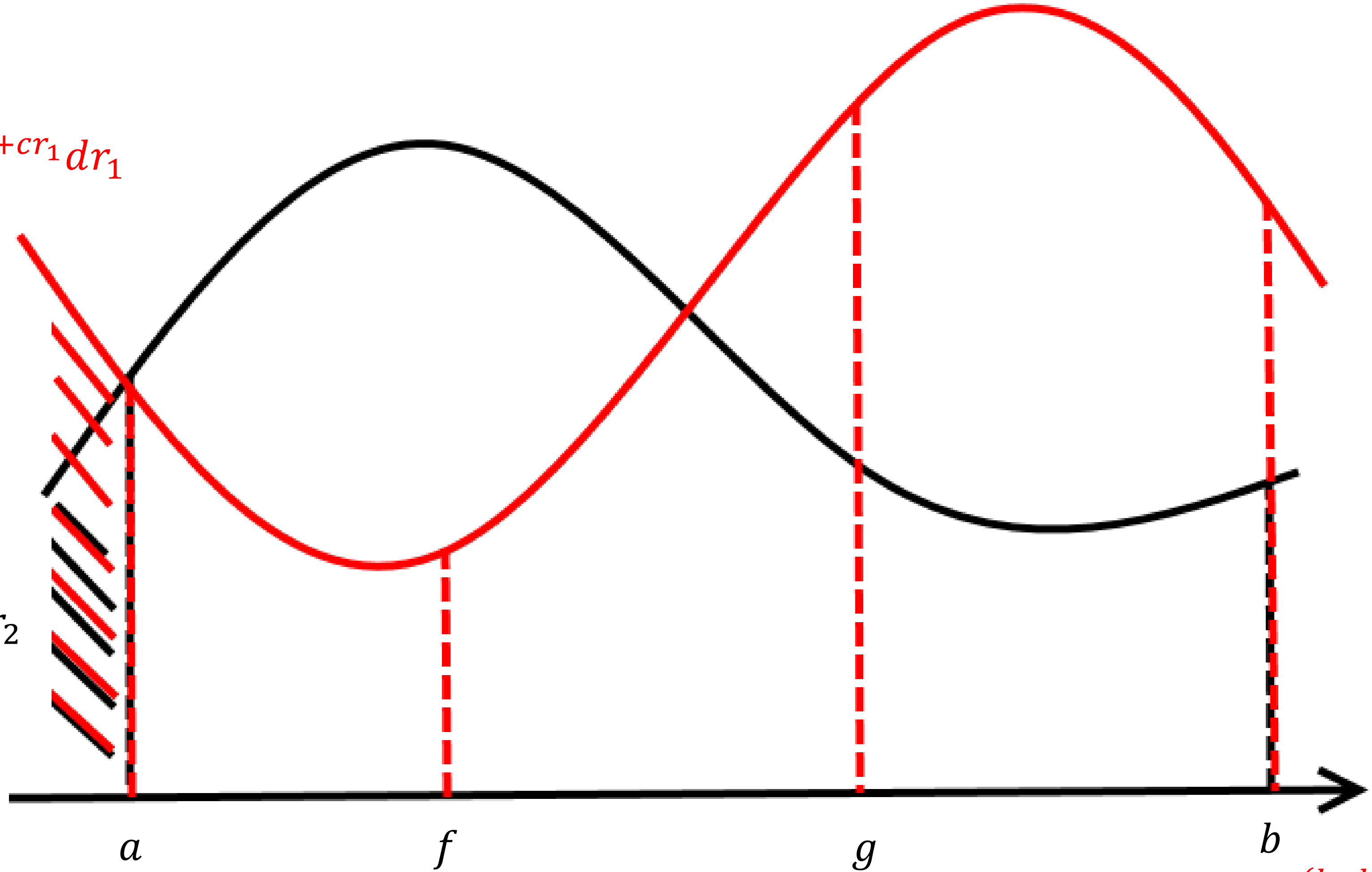


$$e^{-cb}\big(I_1(b) - I_1(a)\big) = w \dots e^{c(f-b)} + w \dots e^{c(g-b)} + w \dots e^{c(b-b)}$$

Solution: Integral over r_1 increases exponentially

$$e^{-ca} I_1(a) = e^{-ca} \int_0^a \dots e^{+cr_1} dr_1$$

$$I_2(a) = \int_0^a \dots e^{-cr_2} I_1(r_2) dr_2$$



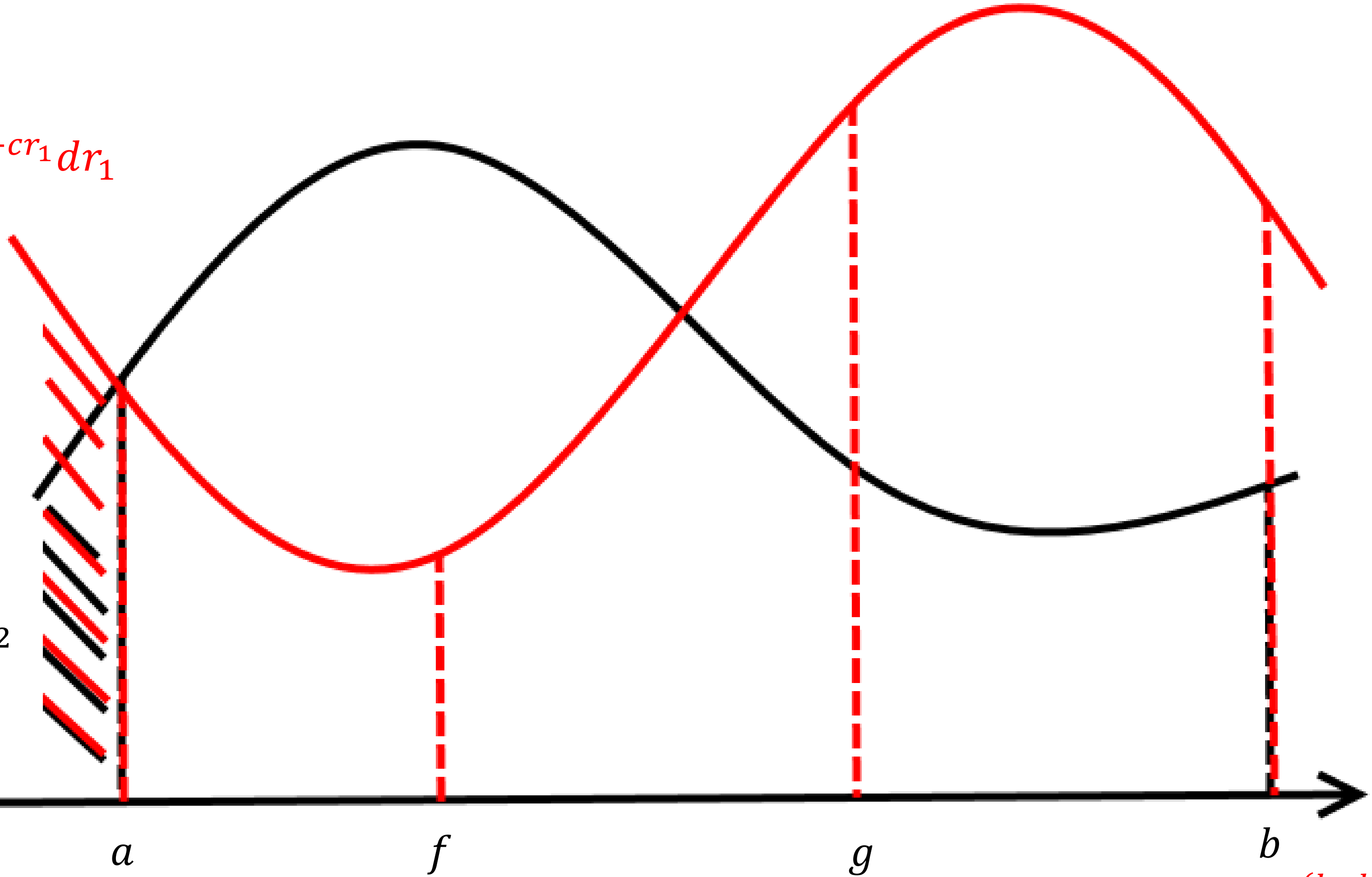
$e^{-cb}\big(I_1(b) - I_1(a)\big) =$ $w \dots e^{c(f-b)}$ $+w \dots e^{c(g-b)}$ $+w \dots e^{c(b-b)}$

$$e^{-cb} I_1(b) = e^{-cb}\big(I_1(b) - I_1(a)\big) + e^{c(a-b)}\left(e^{-ca} I_1(a)\right)$$

Solution: Integral over r_1 increases exponentially

$$e^{-ca} I_1(a) = e^{-ca} \int_0^a \dots e^{+cr_1} dr_1$$

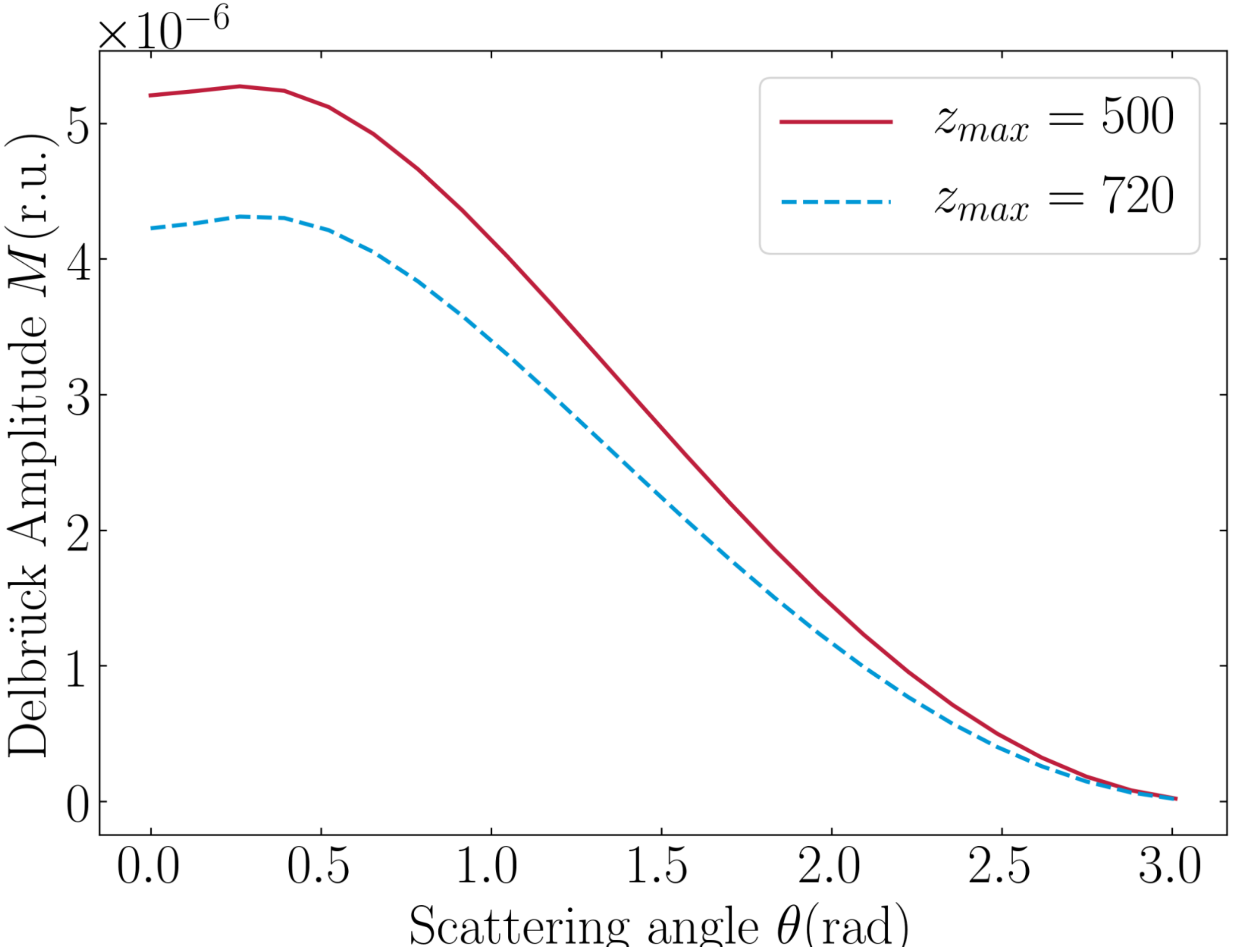
$$I_2(a) = \int_0^a \dots e^{-cr_2} I_1(r_2) dr_2$$



$$e^{-cb}\big(I_1(b) - I_1(a)\big) = \quad w \dots e^{c(f-b)} \quad +w \dots e^{c(g-b)} \quad +w \dots e^{c(b-b)}$$

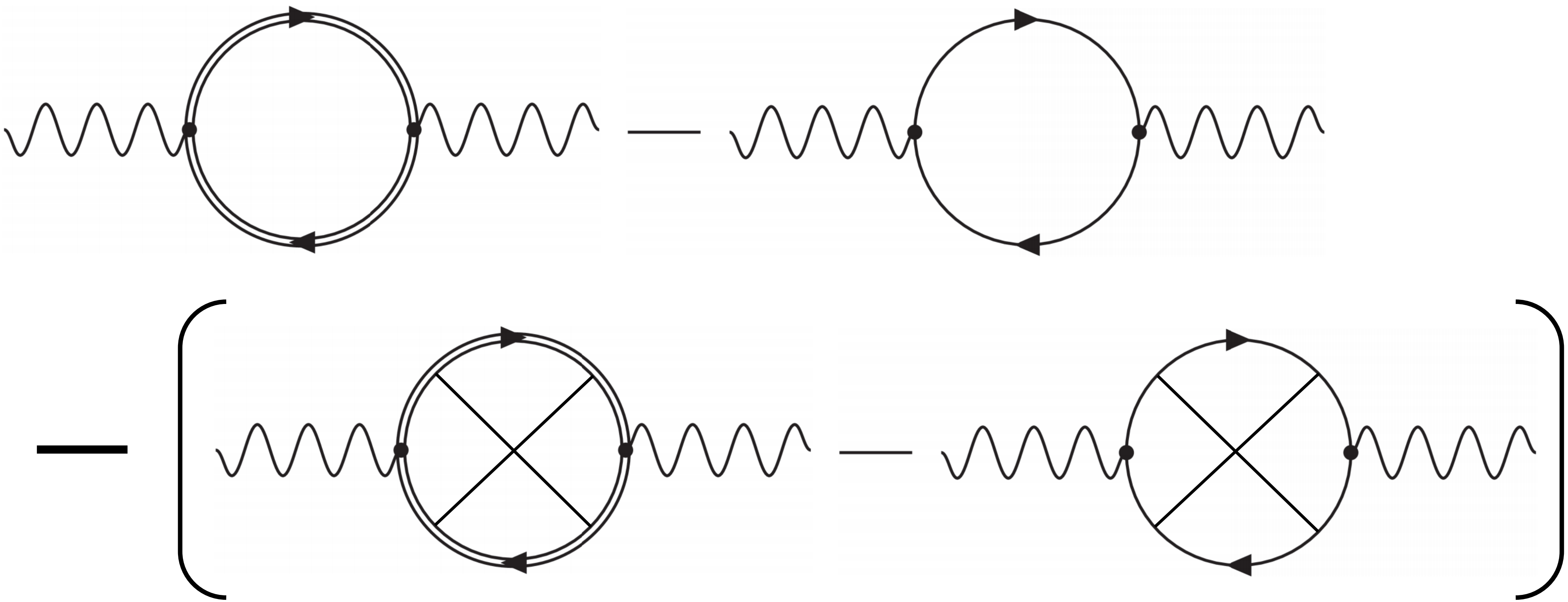
$$e^{-cb} I_1(b) = e^{-cb}\big(I_1(b) - I_1(a)\big) + e^{c(a-b)}\big(e^{-ca} I_1(a)\big) \quad \Rightarrow I_2(b)$$

Results $Z = 10, \omega = 0.5$

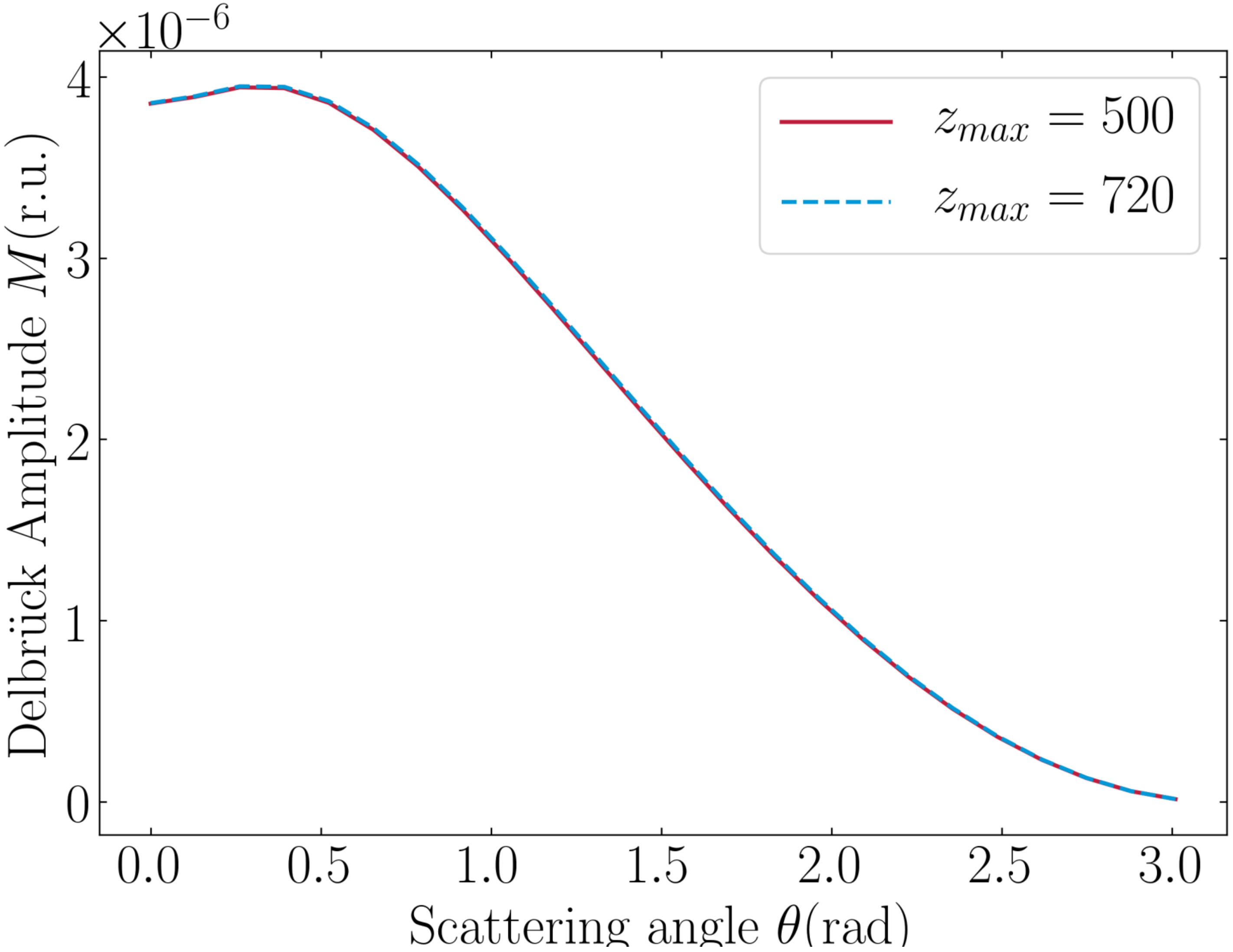


Renormalization

To enhance the numerical convergence, we subtract the non-gauge invariant spurious terms (?) :



Results $Z = 10, \omega = 0.5$



Next objective: Above treshold calculations

Few optimizations to reduce computation time:

- Less integration points for the z‘ integration

N intervals for z‘ integration from 0 to z_{max}

One interval from 0 to A and from A to infinity by change of variabels $x \rightarrow A/t$

A = 5, n_GL = 32	A = 10, n_GL = 24
2.470645184740691e-06	2.470645184741872e-06

- Utilize more cores by parallelization of the radial integration
- More effective extrapolation of the infinite sums (?)