From the exact solution for the Schrödinger equation to NLO cross sections

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"*Singularity is almost invariably a clue*" (Sherlock Holmes)

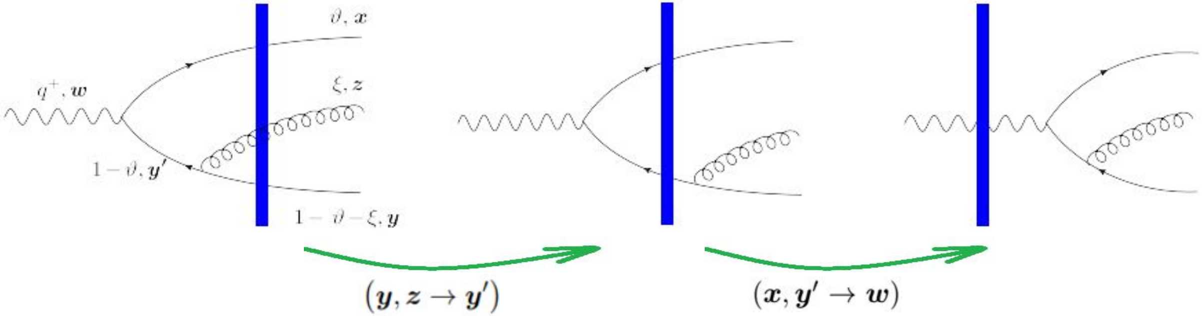
How it all have started?

- ***The initial project***: computing the virtual NLO cross section for dijet (inclusive / diffractive) production.

- ***Previous knowledge***:

1) In the work (with E. Iancu) "***Dihadron production in DIS at NLO: the real corrections***" it has been observed that an elegant pattern appears for amplitudes:

$$\left|\gamma_T^i(Q,q^+,\boldsymbol{w})\right\rangle^{\rm reg}_{q\bar{q}g} = -\frac{e e_f g\, q^+}{2(2\pi)^4}\int_{\boldsymbol{x},\boldsymbol{y},\boldsymbol{z}}\int_0^1 d\vartheta\int_0^{1-\vartheta} d\xi\,\frac{\vartheta}{\sqrt{\xi}}\,\frac{\boldsymbol{R}^j\boldsymbol{Y}^n}{\boldsymbol{Y}^2}\,\delta^{(2)}(\boldsymbol{w}-\boldsymbol{c})$$
$$\times\left\{\Phi^{ijmn}_{\lambda_1\lambda_2}(\vartheta,\xi)\,\frac{Q\,\mathrm{K}_1(QD)}{D}\left[U^{ab}(\boldsymbol{z})V(\boldsymbol{x})t^bV^\dagger(\boldsymbol{y})-t^a\right]_{\alpha\beta}-(\boldsymbol{y},\boldsymbol{z}\to\boldsymbol{y}')\right\}$$



2) JIMWLK should appear already at the amplitude level.

3) The poles can be interpreted as the physical spectrum of the theory.

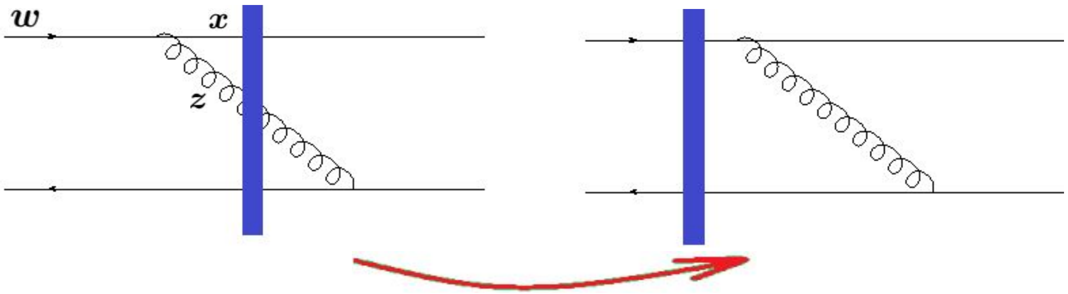
Opening Pandora's box

In practice, the calculation based on *U* leads to one contribution for which these properties **were missing** (!):

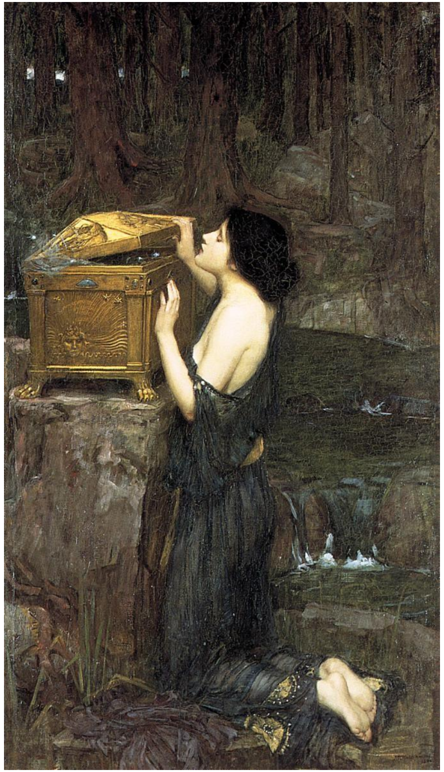
1) *The elegant pattern did not appear.*
2) *JIMWLK could not be observed at the amplitude level.*
3) *There were multiple poles for degenerate configurations.*

All that happened due to one (sub-)contribution:

Two WW fields (simple pole) ***Branch-cut (multiple poles)***



$(x, z \to w)$ **Not working!**



The Schrödinger Equation

The fundamental equation:

$$i\frac{d}{dt}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle\,, \qquad or \qquad \frac{d\hat{\mathcal{O}}(t,t_0)}{dt} = -i\hat{H}(t)\hat{\mathcal{O}}(t,t_0)$$

Predicts a dynamics which is ***differentiable*** (and therefore ***continuous***) at each moment of the evolution.

- As long as the Hamiltonian involves no time dependence:

$$|\Psi(t)\rangle = \hat{U}(t,t_0)|\Psi(t_0)\rangle\,, \qquad \hat{U}(t,t_0) = e^{-i\hat{H}(t-t_0)}$$

- When time dependence is involved it is customary to use the solution

$$\hat{\mathcal{O}}(t,t_0) = \hat{U}(t,t_0) \equiv \mathrm{T}\exp\left[-i\int_{t_0}^{t} dt'\,\hat{H}(t')\right]$$

Which can also be written in the expanded form as (Dyson series)

$$\hat{U}(t,t_0) = \hat{\mathbf{1}} - i\int_{t_0}^{t} dt'\,\hat{H}(t') - \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t')\,\hat{H}(t'') + \ldots$$

How do we conclude that U is unitary?

- ***Exact unitarity is a crucial property for any valid quantum description.***

Using the Dyson expansion:

$$\hat{U}^\dagger(t,t_0)\,\hat{U}(t,t_0) = \hat{\mathbf{1}} + \left(\int_{t_0}^{t} dt'\,\hat{H}(t')\right)^2 - \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t')\,\hat{H}(t'') - \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t'')\,\hat{H}(t') + \ldots$$

Changing variables:

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t'')\,\hat{H}(t') = \int_{t_0}^{t} dt' \int_{t'}^{t} dt''\,\hat{H}(t')\,\hat{H}(t'')$$

After adding integrals:

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t')\,\hat{H}(t'') + \int_{t_0}^{t} dt' \int_{t'}^{t} dt''\,\hat{H}(t')\,\hat{H}(t'') = \left(\int_{t_0}^{t} dt'\,\hat{H}(t')\right)^2$$

So, at least allegedly, *U* is a unitary operator,

$$\hat{U}^\dagger(t,\,t_0)\,\hat{U}(t,\,t_0) = \hat{\mathbf{1}}$$

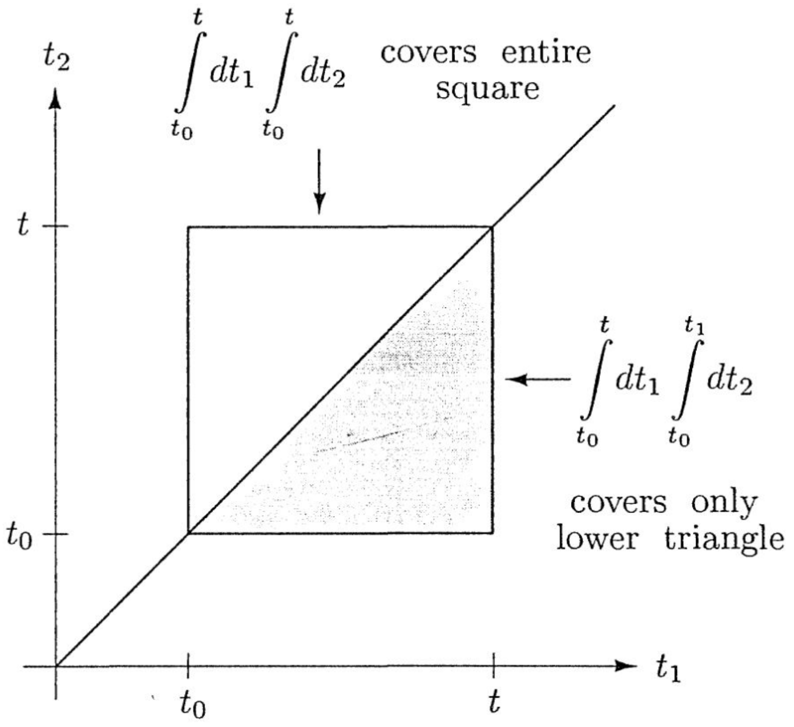


Figure 4.1. Geometric interpretation of Eq. (4.21).

From Peskin and Schroeder, P. 85.

The underlying assumptions

1) ***Linearity***:

$$\int_{t_0}^{t} dt'\, f(t') + \int_{t_0}^{t} dt'\, g(t') = \int_{t_0}^{t} dt'\, \left(f(t') + g(t')\right)$$

2) ***Changing order of integrations (Fubini theorem)***:

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, f(t', t'') = \int_{t_0}^{t} dt' \int_{t'}^{t} dt''\, f(t', t'')$$

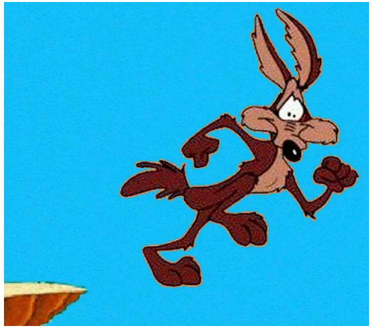
3) ***Adding integration intervals (additivity)***:

$$\int_{t_0}^{t'} dt''\, f(t'') + \int_{t'}^{t} dt''\, f(t'') = \int_{t_0}^{t} dt''\, f(t'')$$

4) ***Exact Hermiticity of the Hamiltonian***:

$$H^\dagger(t) = H(t)$$

Unitarity for distributions, personal perspective:



- Properties 1), 2) and 3) are ***valid*** for Hamiltonians expressed by ***functions***.
- Properties 2) and 3) are ***not valid*** for ***distributions***.

Linearity

Function: an object which assign exactly one ***defined*** (finite) element from a set *Y* to each element of set *X*.

- ***Example***: $f(x) = \frac{1}{x-a}$ is a function defined on the union of two intervals $(-\infty, a) \cup (a, \infty)$, but is ***NOT*** a function on an interval that contains $x = a$.

- ***What happens to linearity for intervals which cross the singularity point?***

```
FullSimplify[Integrate[x / (x - a), {x, -1, 1}] + Integrate[-a / (x - a), {x, -1, 1}]]
```

```
2 + a (-Log[-1 - a] + Log[1 - a] - Log[-1 + a] + Log[1 + a]) if Re[a] > 1 || Re[a] < -1 || a ∉ ℝ
```
$= 2 + a\log(-1)$

```
FullSimplify[Integrate[1, {x, -1, 1}]]
```

2

By using complex deformation (rotating the pole aside):

$$f(x) = \frac{1}{x-a} \quad \longrightarrow \quad O(x) = \frac{1}{x - ae^{i\epsilon}}$$

For ϵ finite, *O(x)* is just a general complex function. For ϵ taken to 0, *O(x)* is a sum of a function and distribution (*Sokhotski-Plemelj theorem*):

$$\lim_{\epsilon \to 0} O(x) = \lim_{\epsilon \to 0} \frac{1}{x - a - i\epsilon} = P.v. \left(\frac{1}{x-a} \right) + i\pi\delta(x-a)$$

Including ϵ is equivalent to adding ***imaginary distribution*** (introducing a discontinuity).

Preliminaries in Analysis

Absolute convergence:

Both $\sum_n a_n$ and $\sum_n |a_n|$ converges, alternatively, both $\int f(x)$ and $\int |f(x)|$.

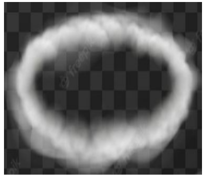
Conditional convergence:

$\sum_n a_n$ converges but not $\sum_n |a_n|$, alternatively $\int f(x)$ converges but not $\int |f(x)|$.

- ***Riemann series theorem***: "*if an infinite series of real numbers is conditionally convergent, then its terms can be arranged in a permutation so that the new series converges to an arbitrary real number, or diverges.*"

- ***Conclusion***: conditionally convergent contributions are ***very fragile***.


Absolute conv.

Conditionally conv.

The Fubini Theorem

Exchanging the ordering of integrations is allowed only for absolute convergent integrals.

$$\int dx \left(\int dy\, f(x,y) \right) = \int dy \left(\int dx\, f(x,y) \right) \quad \textbf{if} \quad \int dx \int dy\, |f(x,y)| < \infty$$

- Example:

$$\int_0^2 \left(\int_0^1 \frac{xy(x^2-y^2)}{(x^2+y^2)^3}\, dy \right) dx = -\frac{1}{20} \qquad \int_0^1 \left(\int_0^2 \frac{xy(x^2-y^2)}{(x^2+y^2)^3}\, dx \right) dy = \frac{1}{5}$$

Check: "***Fubini Counterexample (full version)***" @ *Dr Payam* (youtube).

- Distributions typically ***do not allow*** to exchange the ordering of integrations:

```
Integrate[(2 y - 3) DiracDelta[x - y - 1], {y, 0, t}, {x, y, t}]

(-4 + t) (-1 + t) HeavisideTheta[-1 + t] if t ∈ ℝ

Integrate[(2 y - 3) DiracDelta[x - y - 1], {y, 0, t}, {x, 0, y}]

0
```

For Y.M. theories, the terms of the perturbative expansion are usually divergent before regularization and ***conditionally convergent*** afterwards (but not absolutely convergent).

- ***The simplifications for establishing unitarity are not always valid!***

Additivity

Additivity ***does not hold*** for distributions:

$$\int_{t_0}^{t'} dt''\, f(t'')\delta(t''-t_1) + \int_{t'}^{t} dt''\, f(t'')\delta(t''-t_1) \neq \int_{t_0}^{t} dt''\, f(t'')\delta(t''-t_1)$$

Since the if t_1 coincide with t' the integral may regarded as '*badly defined*', or the distribution considered to *contribute twice*.

```
FullSimplify[Integrate[f (t') * DiracDelta[t' - a], {t', 0, t1}] + Integrate[f (t') * DiracDelta[t' - a], {t', t1, t}], Assumptions → t > 0]
```

```
a f ((-1 + 2 HeavisideTheta[t1]) HeavisideTheta[a - t1 HeavisideTheta[-t1]] HeavisideTheta[-a + t1 HeavisideTheta[t1]] + (-1 + 2 HeavisideTheta[t - t1])
    HeavisideTheta[a - t1 HeavisideTheta[t - t1] - t HeavisideTheta[-t + t1]] HeavisideTheta[-a + t HeavisideTheta[t - t1] + t1 HeavisideTheta[-t + t1]]) if a ∈ ℝ && t1 ∈ ℝ
```

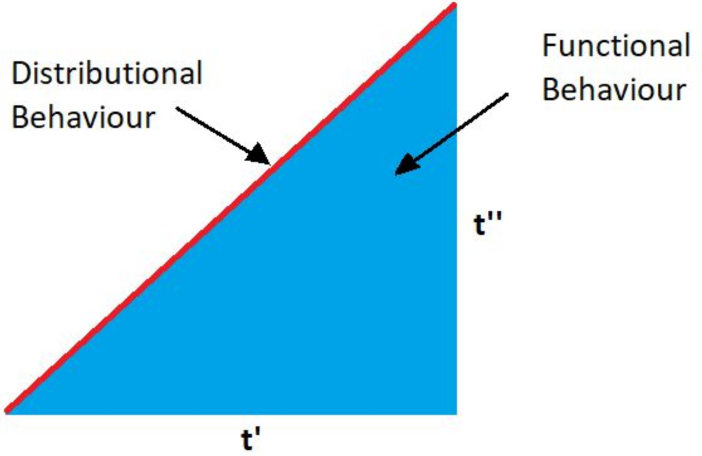
```
FullSimplify[Integrate[f (t') * DiracDelta[t' - a], {t', 0, t}], Assumptions → t > 0]
```

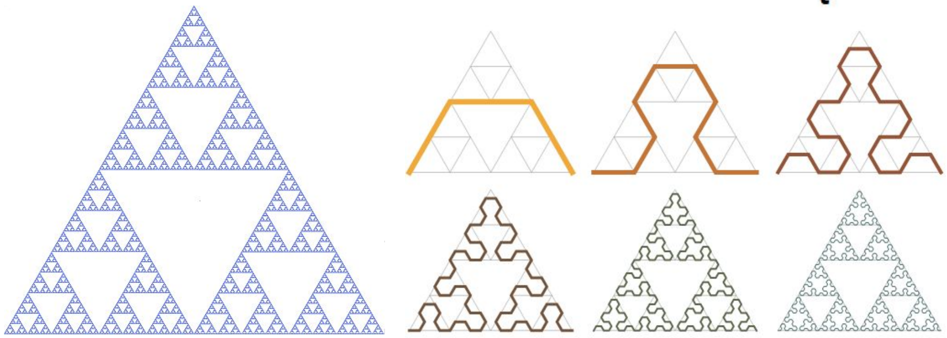
```
a f HeavisideTheta[a, -a + t] if a ∈ ℝ
```

- Check: "*When functions have no value(s)*" by Steven G. Johnson.

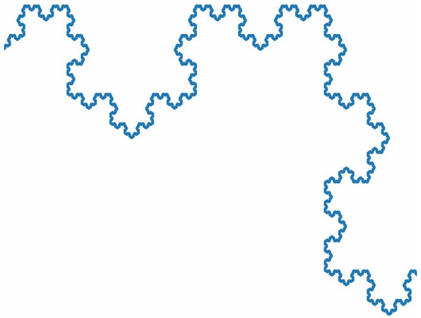
What is measure-0?

The discrete part of the evolution lives on the boundary of the integration triangle (measure-0 line).





Sierpinski triangle



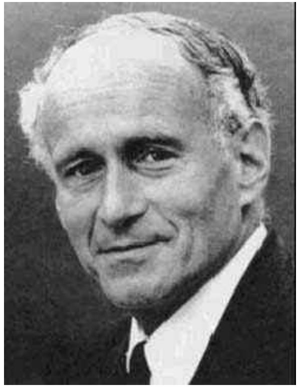
Koch snowflake

Pharoh's dream

Handling distributions with Dyson series

A hint on the incapability of the Dyson series to cope with distributions is evident since it involves a measure-0 direct product of two Hamiltonians (contact term).

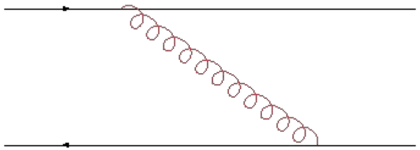
$$\hat{U}(t,t_0) = \hat{\mathbf{1}} - i\int_{t_0}^{t} dt'\,\hat{H}(t') - \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t')\,\hat{H}(t'') + \dots$$



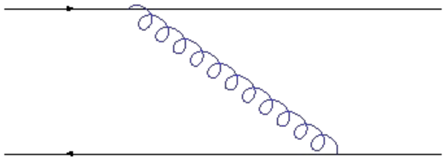
The square of a distribution cannot be defined consistently:
"***L. Schwartz, Sur l'impossibilité de la multiplication des distributions***".

It is crucial to understand that this issue is ***unrelated with UV divergences*** and cannot be cured by regularization procedure.

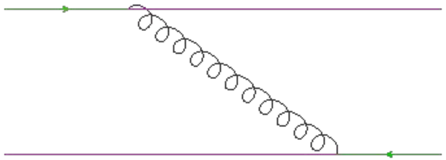
- Check: "*Causal perturbation theory*" by G. Scharf.



UV (high energy gluon), treated via dimreg



IR (soft or collinear gluon)



Degeneracy: regardless of the gluon eigenvalue (measure-0 options)

On the "Pitaron"

A unitarized version of *U* can be found by multiplying *U* by an additional operator:

$$\hat{\mathcal{P}}(t,\, t_0) \;\equiv\; \hat{\mathcal{N}}(t,\, t_0)\,\hat{U}(t,\, t_0)$$

With the Hermitian normalization operator:

$$\hat{\mathcal{N}}(t,\, t_0) \;\equiv\; \sqrt{\hat{U}^{\dagger -1}(t,\, t_0)\,\hat{U}^{-1}(t,\, t_0)}$$

Note that unitarity is **manifest** (unbreakable):

$$\hat{\mathcal{P}}^{\dagger}(t,\, t_0)\,\hat{\mathcal{P}}(t,\, t_0) \;=\; \hat{U}^{\dagger}(t,\, t_0)\,\hat{U}^{\dagger -1}(t,\, t_0)\,\hat{U}^{-1}(t,\, t_0)\,\hat{U}(t,\, t_0) \;=\; \hat{\mathbf{1}}$$

Regardless of the choice of Hamiltonian.

Wider class of exotic quantum field theories, in which unitarity is proven to be broken, can now be studies normally, such as QFT with ***open systems***, ***fractional dimensions*** or ***non-commutative spaces***.

How to take a square root?

The square root of a matrix extends the notion of square root from numbers to matrices. A matrix B is said to be a square root of A if the matrix product BB is equal to A.

- Hermitian operators can always be diagonalized with real entries on the diagonal, and therefore always have a square root.

$$\mathcal{N}_q^2 = a^2 \left|q\right\rangle \left\langle q\right| + b^2 \left|qg\right\rangle \left\langle qg\right| \longrightarrow \mathcal{N}_q = \pm a \left|q\right\rangle \left\langle q\right| \pm b \left|qg\right\rangle \left\langle qg\right|$$

- A unique result is obtained by using the initial conditions.

The Schrodinger-Liouville's unification

Let us see that P solves the Schrodinger equation:

$$\frac{d\hat{\mathcal{P}}(t,\,t_0)}{dt} = -i\hat{H}(t)\hat{\mathcal{P}}(t,\,t_0)$$

According to Leibniz product rule:

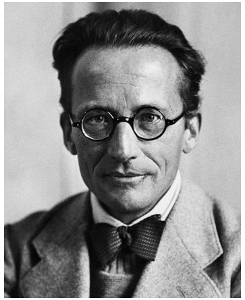
$$\frac{d\hat{\mathcal{P}}(t,\,t_0)}{dt} = \hat{\mathcal{N}}(t,\,t_0)\frac{d\hat{U}(t,\,t_0)}{dt} + \frac{d\hat{\mathcal{N}}(t,\,t_0)}{dt}\hat{U}(t,\,t_0)$$

$$\left[\hat{H}(t),\,\hat{\mathcal{N}}(t,\,t_0)\right] + \hat{\mathcal{N}}(t,\,t_0)\hat{H}(t) = \hat{H}(t)\hat{\mathcal{N}}(t,\,t_0)$$

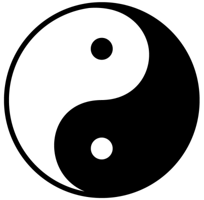
We arrive at:

$$\hat{\mathcal{N}}(t,t_0)\left\{\frac{d\hat{U}(t,t_0)}{dt} + i\hat{H}(t)\hat{U}(t,t_0)\right\} = \left\{\frac{d\hat{\mathcal{N}}(t,t_0)}{dt} + i\left[\hat{H}(t),\,\hat{\mathcal{N}}(t,t_0)\right]\right\}\hat{U}(t,t_0)$$

Implying "two equations at once":



$$\frac{d\hat{U}(t,\,t_0)}{dt} = -i\hat{H}(t)\hat{U}(t,\,t_0) \qquad \frac{d\hat{\mathcal{N}}(t,\,t_0)}{dt} = -i\left[\hat{H}(t),\,\hat{\mathcal{N}}(t,\,t_0)\right]$$



Generalizing the Magnus expansion

Since P is an exact unitary operator it can be written ***without*** the time-ordering "**T** operator":

$$\hat{\mathcal{P}}(t,\, t_0) \,=\, e^{-i\hat{\Omega}(t,t_0)} \qquad\qquad \Omega(t,\, t_0) \,=\, \int_{t_0}^{t} dt'\, \hat{H}(t') \,-\, \frac{i}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \left[\hat{H}(t'),\, \hat{H}(t'')\right]$$

Computing the inverse:

$$\hat{U}^{-1}(t,t_0) \,=\, \hat{\mathbf{1}} + i\int_{t_0}^{t} dt'\, \hat{H}(t') - \left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^2 + \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \hat{H}(t')\, \hat{H}(t'') + \ldots$$

Then:

$$\hat{\mathcal{N}}(t,\, t_0) \,=\, \hat{\mathbf{1}} \,-\, \frac{1}{2}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^2 \,+\, \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \left\{\hat{H}(t'),\, \hat{H}(t'')\right\} \,+\, \ldots$$

One arrives at:

$$\hat{\mathcal{P}}(t,\, t_0) \,=\, \hat{\mathbf{1}} \,-\, i\int_{t_0}^{t} dt'\, \hat{H}(t') \,-\, \frac{1}{2}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^2 \,-\, \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \left[\hat{H}(t'),\, \hat{H}(t'')\right] \,+\, \ldots$$

"*On the Exponential Solution of Differential Equations for a Linear Operator*" by Wilhelm Magnus (1954). ***With this expansion the anticipated JIMWLK structure is restored!***

N via Truncation

There are several different ways in which the operator *N* can get a non-trivial value.

A trivial demonstration is via truction of the perturbative expansion at first order, assuming **nilpotent Hamiltonian** or **negligible correction at order g^2**:

$$\left\| \int_{t_0}^{t} dt' \, \hat{H}(t') \right\| \gg \left\| \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \, \hat{H}(t') \, \hat{H}(t'') \right\|$$

In these cases only one term should be kept:

$$\hat{U}(t, t_0) \approx \hat{\mathbf{1}} - i \int_{t_0}^{t} dt' \, \hat{H}(t')$$

The operator *N* can be computed via

$$\hat{\mathcal{N}}(t, t_0) = \left(\sqrt{\hat{U}(t, t_0) \, \hat{U}^{\dagger}(t, t_0)} \right)^{-1}$$

Assuming Hermiticity, leads to:

$$\hat{\mathcal{N}}(t, t_0) \approx \hat{\mathbf{1}} - \frac{1}{2} \left\| \int_{t_0}^{t} dt' \, \hat{H}(t') \right\|$$

Breaking unitarity in QM

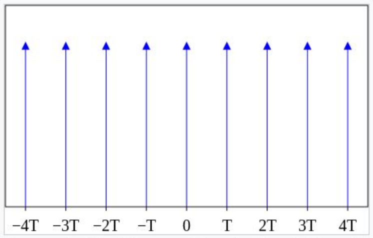
Dirac comb

文A 12 languages

In mathematics, a **Dirac comb** (also known as **shah function**, **impulse train** or **sampling function**) is a periodic function with the formula

$$Ш_{T}(t) := \sum_{k=-\infty}^{\infty} \delta(t-kT)$$

for some given period T.[1] Here *t* is a real variable and the sum extends over all integers *k*. The Dirac delta function δ and the Dirac comb are tempered distributions.[2][3] The graph of the function resembles a comb (with the δs as the comb's *teeth*), hence its name and the use of the comb-like Cyrillic letter sha (Ш) to denote the function.



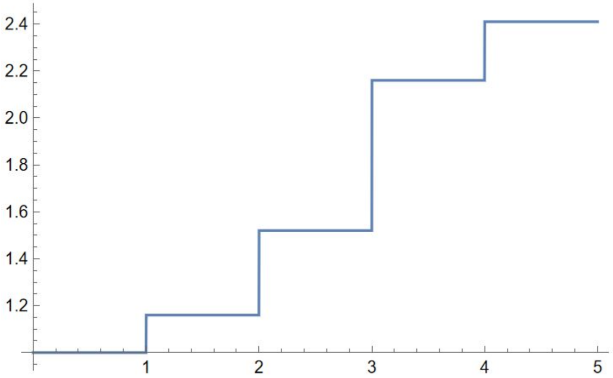
The graph of the Dirac comb function is an infinite series of Dirac delta functions spaced at intervals of T

$$\hat{U}^{\dagger}(t,t_0)\,\hat{U}(t,t_0) = \hat{1} + \left(\int_{t_0}^{t} dt'\,\hat{H}(t')\right)^2 - \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t')\,\hat{H}(t'') - \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t'')\,\hat{H}(t') + \ldots$$

```
H[t_] = 0.4*DiracDelta[t - 1] + 0.6*DiracDelta[t - 2] + 0.8*DiracDelta[t - 3] + 0.5*DiracDelta[t - 4]
0.5 DiracDelta[-4 + t] + 0.8 DiracDelta[-3 + t] + 0.6 DiracDelta[-2 + t] + 0.4 DiracDelta[-1 + t]

f[t_] := 1 + Integrate[H[t1]*H[t2], {t1, 0, t}, {t2, 0, t}] - 2 Integrate[H[t1]*H[t2], {t1, 0, t}, {t2, 0, t1}]

Plot[f[t], {t, 0, 5}]
```



The world of Hamiltonians

- ***Regular***

Hermitian Hamiltonian with '*functional entries*' and therefore contain no singularities. No poles or distributions are involved.

$$\hat{U}^\dagger(t,\, t_0)\frac{d\hat{U}(t,\, t_0)}{dt} = -i\hat{U}^\dagger(t,\, t_0)\hat{H}(t)\hat{U}(t,\, t_0), \qquad \frac{d\hat{U}^\dagger(t,\, t_0)}{dt}\hat{U}(t,\, t_0) = i\hat{U}^\dagger(t,\, t_0)\hat{H}(t)\hat{U}(t,\, t_0)$$

$$\frac{d}{dt}\left(\hat{U}^\dagger(t,\, t_0)\hat{U}(t,\, t_0)\right) = 0 \qquad \longrightarrow \qquad \hat{U}^\dagger(t,\, t_0)\hat{U}(t,\, t_0) = const$$

- ***Singular***

Hamiltonian that contain at least one point of singularity as distributions or $\hat{H}(t) = \frac{t-t_1}{(t-t_1)^2-\Delta^2}\hat{\mathbf{1}}$
Singular Hamiltonians break the unitarity of *U* (but not of *P*) for a certain intervals.

$$\hat{U}^\dagger(t,\, t_0)\hat{U}(t,\, t_0)\Big|_{-\infty<t_0\leq t<t_1+|\Delta|-\epsilon} = \hat{\mathbf{1}}, \qquad \hat{U}^\dagger(t,\, t_0)\hat{U}(t,\, t_0)\Big|_{t_1+|\Delta|-\epsilon<t_0\leq t<t_1+|\Delta|+\epsilon} \neq \hat{\mathbf{1}}.$$

$$\hat{U}^\dagger(t,\, t_0)\hat{U}(t,\, t_0)\Big|_{t_1+|\Delta|+\epsilon<t_0\leq t<\infty} = \hat{\mathbf{1}},$$

- ***Non-Hermitian Hamiltonians***

Generalization which allows us to study the singular case by taking a limit (***carefully***).

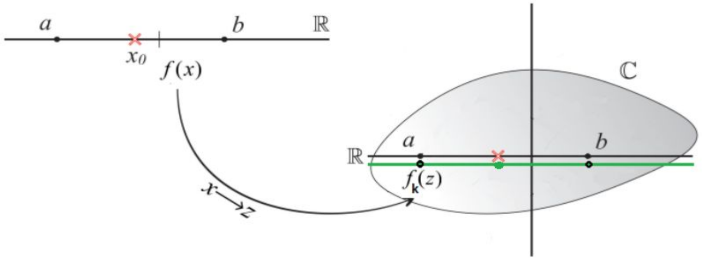
How to perform complex deformations?

The pole becomes a winding/portal point via the complexification

$$\hat{H}(t) \in \mathbb{R} \longrightarrow \hat{H}(z) \in \mathbb{C}$$

If the complex limit exist, one can interpret it as the original Hamiltonian:

$$\lim_{Im\, z \to 0} \hat{H}(z) = \hat{H}(t).$$



- *In order for a complex limit to exist, each way in which z can approach z_0 must yield the same limiting value.*

$$\hat{\mathcal{N}}(t, t_0) = \hat{\mathbf{1}} - \frac{1}{2}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^{\dagger} \int_{t_0}^{t} dt'\, \hat{H}(t') + \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \hat{H}(t')\, \hat{H}(t'') + \frac{1}{2}\left(\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \hat{H}(t')\, \hat{H}(t'')\right)^{\dagger} + \ldots$$

$$\hat{\mathcal{P}}(t, t_0) = \hat{\mathbf{1}} - i\int_{t_0}^{t} dt'\, \hat{H}(t') - \frac{1}{2}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^{\dagger}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)$$
$$- \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \hat{H}(t')\, \hat{H}(t'') + \frac{1}{2}\left(\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \hat{H}(t')\, \hat{H}(t'')\right)^{\dagger} + \ldots$$

An example in QM

Let us look on the case of a free particle subject for two kinds of perturbations:

$$H_0(t) = \frac{p^2}{2m}, \qquad H(t) = \frac{g}{\Delta}\left(\sin(\omega(t-t_1))\hat{\sigma}_2 + \hat{\sigma}_3\right),$$
$$H_0(t) = \frac{p^2}{2m}, \qquad H(t) = g\frac{t-t_1}{(t-t_1)^2-\Delta^2}\hat{\mathbf{1}}.$$

One note that the first perturbation keep unitarity exact:

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \sin(\omega(t'-t_1))\sin(\omega(t''-t_1)) = \int_{t_0}^{t} dt' \int_{t'}^{t} dt''\, \sin(\omega(t'-t_1))\sin(\omega(t''-t_1))$$
$$= \frac{1}{2\omega^2}\left(\cos(\omega(t_1-t_0)) - \cos(\omega(t-t_1))\right)^2.$$

This is no longer valid for the singular Hamiltonian. In order to study a singular Hamiltonian we study a larger class of non-hermitian Hamiltonians:

$$\hat{H}(t) = g\frac{t-t_1}{(t-t_1)^2-\Delta^2}\hat{\mathbf{1}} \quad \longrightarrow \quad \hat{H}(t,\, i\epsilon) = g\frac{t-t_1}{(t-t_1)^2-\Delta^2-i\epsilon}\hat{\mathbf{1}}$$

The original dynamics is obtained as a private case of a vanishing deformation:

$$\hat{H}(t) = \lim_{\epsilon\to 0}\hat{H}(t,\, i\epsilon)$$

By Sokhotski-Plemelj theorem:

$$\frac{1}{(t'-t_0)^2-\Delta^2-i\epsilon} = P.v.\frac{1}{(t'-t_0)^2-\Delta^2} + i\pi\delta((t'-t_0)^2-\Delta^2)$$

The product is given by:

$$H^\dagger(t')H(t'') = \frac{t'-t_1}{(t'-t_1)^2-\Delta^2+i\epsilon}\frac{t''-t_1}{(t''-t_1)^2-\Delta^2-i\epsilon} = (t'-t_1)(t''-t_1)\left(f_1(t',t'')+i\pi g_1(t',t'')\right)$$

With:

$$f_1(t',t'') \equiv P.v.\frac{1}{(t'-t_0)^2-\Delta^2}\,P.v.\frac{1}{(t''-t_0)^2-\Delta^2} + \pi^2\delta((t'-t_0)^2-\Delta^2)\delta((t''-t_0)^2-\Delta^2),$$

$$g_1(t',t'') \equiv P.v.\frac{1}{(t'-t_0)^2-\Delta^2}\delta((t''-t_0)^2-\Delta^2) - P.v.\frac{1}{(t''-t_0)^2-\Delta^2}\delta((t'-t_0)^2-\Delta^2).$$

Similarly,

$$H(t')H(t'') = \frac{t'-t_1}{(t'-t_1)^2-\Delta^2-i\epsilon}\frac{t''-t_1}{(t''-t_1)^2-\Delta^2-i\epsilon} = (t'-t_1)(t''-t_1)\left(f_2(t',t'')+i\pi g_2(t',t'')\right)$$

with:

$$f_2(t',t'') \equiv P.v.\frac{1}{(t'-t_0)^2-\Delta^2}\,P.v.\frac{1}{(t''-t_0)^2-\Delta^2} - \pi^2\delta((t'-t_0)^2-\Delta^2)\delta((t''-t_0)^2-\Delta^2),$$

$$g_2(t',t'') \equiv P.v.\frac{1}{(t'-t_0)^2-\Delta^2}\delta((t''-t_0)^2-\Delta^2) + P.v.\frac{1}{(t''-t_0)^2-\Delta^2}\delta((t'-t_0)^2-\Delta^2).$$

$$\hat{\mathcal{N}}(t,t_0) = \hat{\mathbf{1}} - \frac{1}{2} g^2\pi^2 \left(\int_{t_0}^{t} dt'\,(t'-t_1)\,\delta((t'-t_1)^2-\Delta^2)\right)^2$$
$$- g^2\pi^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,(t'-t_1)(t''-t_1)\,\delta((t'-t_1)^2-\Delta^2)\,\delta((t''-t_1)^2-\Delta^2).$$

$$\hat{\mathcal{N}}(t,t_0) = \hat{\mathbf{1}} - \frac{1}{8} g^2\pi^2\, Boole\,[t_0 < -\Delta + t_1 < t \,||\, t < -\Delta + t_1 < t_0]$$

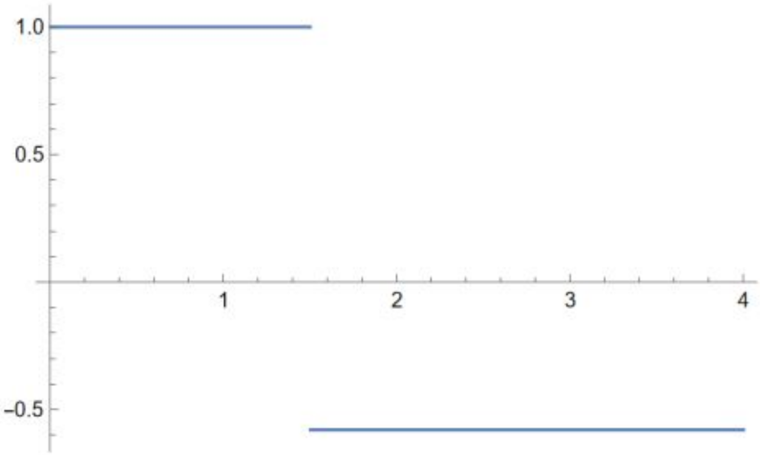


Figure 4. Plot from mathematica describing the time evolution of $\hat{\mathcal{N}}$ from eq. (4.18) for $t \in [0, 4]$. The following parametrization was used $g = 0.4$, $\Delta = 0.5$, $t_0 = 0$, $t_1 = 1$.

$$H(t) = \frac{t-t_1}{(t-t_1)^2-\Delta^2-i\epsilon} + \frac{t-t_2}{(t-t_2)^2-\Delta^2-i\epsilon}$$

$$\hat{\mathcal{N}}(t,t_0) = \hat{\mathbf{1}} - \frac{1}{2}g^2\pi^2\left(\int_{t_0}^{t} dt' \ \left((t'-t_1)\delta((t'-t_1)^2-\Delta^2) + (t'-t_2)\delta((t'-t_2)^2-\Delta^2)\right)\right)^2$$
$$- g^2\pi^2\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \ \left((t'-t_1)\delta((t'-t_1)^2-\Delta^2) + (t'-t_2)\delta((t'-t_2)^2-\Delta^2)\right)$$
$$\times \left((t''-t_1)\delta((t''-t_1)^2-\Delta^2) + (t''-t_2)\delta((t''-t_2)^2-\Delta^2)\right).$$

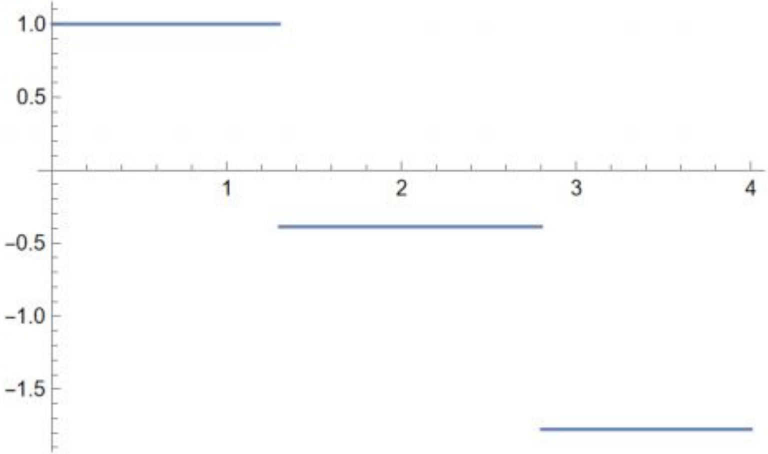


Figure 5. Plot from mathematica describing the time evolution of $\hat{\mathcal{N}}$ from eq. (4.20) for $t \in [0, 4]$. The following parametrization was used $g = 0.6$, $\Delta = 0.8$, $t_0 = 0$, $t_1 = 0.5$, $t_2 = 2$.

Can we really iterate limits?

Iteration of limits is not guaranteed usually, as in the simple example below:

$$\lim_{y\to 0}\lim_{x\to 0}\frac{x^2}{x^2+y^2}=\lim_{y\to 0}0=0, \qquad \lim_{x\to 0}\lim_{y\to 0}\frac{x^2}{x^2+y^2}=\lim_{x\to 0}1=1.$$

$$\lim_{n\to\infty}\int dx\,\frac{1}{\left(1+\frac{x}{n}\right)^n-z}\neq\int dx\,\lim_{n\to\infty}\frac{1}{\left(1+\frac{x}{n}\right)^n-z}=\int dx\frac{1}{e^x-z}$$

the necessary condition to permit that is ***Lebesgue dominated convergence***.

- When using complex deformations, one must be careful to perform the limits in the correct ordering:

$$\int d\Phi_{f,j,i}\lim_{\epsilon\to 0}\frac{1}{E_f-E_i-2i\epsilon}\lim_{\epsilon\to 0}\frac{1}{E_j-E_i-i\epsilon}\neq\lim_{\epsilon\to 0}\int d\Phi_{f,j,i}\frac{1}{E_f-E_i-2i\epsilon}\frac{1}{E_j-E_i-i\epsilon}$$

$$\int\frac{d^d\mathbf{p}}{(2\pi)^d}\lim_{\epsilon\to 0}f(\mathbf{p},\,\epsilon)\neq\lim_{\epsilon\to 0}\int\frac{d^d\mathbf{p}}{(2\pi)^d}f(\mathbf{p},\,\epsilon)$$

QFT = Functions + Distributions

For the asymptotic states, after deformation the order g term of *U* reads:

$$i\int_{-\infty}^{0-} dt'\, H(t',\mathbf{p}) \,=\, i\int_{-\infty}^{0-} dt' \int d\Phi_{f,i} \lim_{\epsilon\to 0} e^{i(E_f-E_i-i\epsilon)t'} \left|f\right\rangle \left\langle f\right| \hat{H}(\mathbf{p}) \left|i\right\rangle \left\langle i\right|$$

After plugging
$H(t,\mathbf{p}) \,=\, e^{i\hat{H}(\mathbf{p})t}\hat{H}(\mathbf{p})e^{-i\hat{H}(\mathbf{p})t}$

- *The time integration commutes with the other operations*:

$$\left[\int_{-\infty}^{0-} dt'\,,\lim_{\epsilon\to 0}\right] = \left[\int_{-\infty}^{0-} dt'\,, \int d\Phi_{f,i}\right] = 0, \qquad \left[\int d\Phi_{f,i},\, \lim_{\epsilon\to 0}\right] \neq 0$$

Then:

$$i\int_{-\infty}^{0-} dt'\, H(t',\mathbf{p}) \,=\, i\int d\Phi_{f,i} \lim_{\epsilon\to 0} \int_{-\infty}^{0-} dt'\, e^{i(E_f-E_i-i\epsilon)t'} \left|f\right\rangle \left\langle f\right| \hat{H}(\mathbf{p}) \left|i\right\rangle \left\langle i\right|$$

Which leads to:

$$i\int_{-\infty}^{0-} dt'\, H(t',\mathbf{p}) \,=\, \int d\Phi_{f,i} \lim_{\epsilon\to 0} \frac{1}{(E_f-E_i-i\epsilon)} \left|f\right\rangle \left\langle f\right| \hat{H}(\mathbf{p}) \left|i\right\rangle \left\langle i\right|$$

By using Sokhotski-Plemelj theorem:

Usually not important due
$x\,\delta(x) = 0$

$$\int_{-\infty}^{0-} dt'\, H(t',\mathbf{p}) \,=\, \int d\Phi_{f,i} \left[P.v.\left(\frac{1}{E_f-E_i}\right) + i\pi\delta(E_f-E_i)\right] \left|f\right\rangle \left\langle f\right| \hat{H}(\mathbf{p}) \left|i\right\rangle \left\langle i\right|$$

One more term

The g^2 terms of *U* reads:

$$\int_{-\infty}^{0-} dt'' \int_{-\infty}^{t''} dt'\, \hat{H}(t'')\, \hat{H}(t') = -\int d\Phi_{f,j,i} \left[\lim_{\epsilon\to 0} \frac{1}{E_f - E_i - 2i\epsilon}\right] \left[\lim_{\epsilon\to 0} \frac{1}{E_j - E_i - i\epsilon}\right]$$
$$\times |f\rangle \langle f| \hat{H}(\mathbf{p}) |j\rangle \langle j| \hat{H}(\mathbf{p}) |i\rangle \langle i| \,,$$

By using Sokhotski-Plemelj theorem:

The non-trivial discontinuities term which is removed by N

$$\delta(f(x)) = \sum_{measure-0\, n} |f'(x_n)|^{-1} \delta(x - x_n)$$

$$\int_{-\infty}^{0-} dt'' \int_{-\infty}^{t''} dt'\, \hat{H}(t'')\, \hat{H}(t') = -\int d\Phi_{f,j,i} \left[P.v. \left(\frac{1}{E_f - E_i}\right) + 2i\pi\delta(E_f - E_i)\right]\left[P.v. \left(\frac{1}{E_j - E_i}\right) + i\pi\delta(E_j - E_i)\right]$$
$$\times |f\rangle \langle f| \hat{H}(\mathbf{p}) |j\rangle \langle j| \hat{H}(\mathbf{p}) |i\rangle \langle i| \,,$$

The normalization operator removes the measure-0 Dirac delta functions:

$$\hat{\mathcal{N}}(0, -\infty) = \hat{\mathbf{1}} - \int d\Phi_{f,j,i}\, 2\pi i\delta(E_f - E_i)\, P.v. \left(\frac{1}{E_j - E_i}\right) |f\rangle \langle f| \hat{H}(\mathbf{p}) |j\rangle \langle j| \hat{H}(\mathbf{p}) |i\rangle \langle i|$$

The g^2 term of *P* expressed **only** via P.v. :

Two terms forming an anti-Hermitian combination

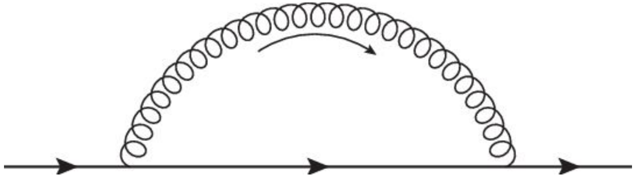
$$\int d\Phi_{f,j,i} \left[\frac{1}{2} P.v. \left(\frac{1}{E_f - E_i}\right) P.v. \left(\frac{1}{E_j - E_i}\right) - \frac{1}{2} P.v. \left(\frac{1}{E_f - E_i}\right) P.v. \left(\frac{1}{E_j - E_f}\right)\right.$$
$$\left. -\frac{1}{2} P.v. \left(\frac{1}{E_f - E_j}\right) P.v. \left(\frac{1}{E_j - E_i}\right)\right] |f\rangle \langle f| \hat{H}(\mathbf{p}) |j\rangle \langle j| \hat{H}(\mathbf{p}) |i\rangle \langle i|$$

Example in QFT

The time ordered exponential, after introducing the Fock space:

$$\hat{U}(0,-\infty)\,|q\rangle = \left(\hat{\mathbf{1}} - \int |q_j g\rangle \lim_{\epsilon\to 0} \frac{\langle q_j g|\,\hat{H}\,|q_i\rangle}{E_{q_j g} - E_{q_i} - i\epsilon} \langle q_i| + \int |q_f\rangle \lim_{\epsilon\to 0} \frac{\langle q_f|\,\hat{H}\,|q_j g\rangle}{\boxed{(E_{q_f} - E_{q_i} - i\epsilon)}} \lim_{\epsilon\to 0} \frac{\langle q_j g|\,\hat{H}\,|q_i\rangle}{(E_{q_j g} - E_{q_i} - i\epsilon)} \langle q_i| \right) |q\rangle$$

The "quark self-energy" has a '*badly defined*' energy denominator.
Wrongly, assumed to be treated via combining with its (c.c.) amplitude.



The solution is to rescale via introducing the "***WF normalization***" or "***LSZ factor***",

$$\hat{U}(0,-\infty)\,|q\rangle \longrightarrow Z\,\hat{U}(0,-\infty)\,|q\rangle$$

And extract ***Z*** by demanding unitarity,

$$|Z|^2 \,\langle q|\,\hat{U}^\dagger(0,-\infty)\hat{U}(0,-\infty)\,|q\rangle = 1 \quad\longrightarrow\quad |Z|^2 = \frac{1}{\langle q|\,\hat{U}^\dagger(0,-\infty)\hat{U}(0,-\infty)\,|q\rangle} = \langle q|\,\hat{\mathcal{N}}^2(0,-\infty)\,|q\rangle$$

Reproducing via N

Keeping only the relevant terms, the following expansion for *N* is obtained:

$$\hat{\mathcal{N}}(0,-\infty) = \hat{\mathbf{1}} - \int |q_f\rangle \lim_{\epsilon\to 0} \frac{\langle q_f|\,\hat{H}\,|q_j g\rangle}{(E_{q_f} - E_{q_i} - i\epsilon)} \lim_{\epsilon\to 0} \frac{\langle q_j g|\,\hat{H}\,|q_i\rangle}{(E_{q_j g} - E_{q_i} - i\epsilon)} \langle q_i|$$

$$-\frac{1}{2}\int |q_f\rangle \lim_{\epsilon\to 0} \frac{\langle q_f|\,\hat{H}\,|q_j g\rangle}{(E_{q_j g} - E_{q_f} + i\epsilon)} \lim_{\epsilon\to 0} \frac{\langle q_j g|\,\hat{H}\,|q_i\rangle}{(E_{q_j g} - E_{q_i} - i\epsilon)} \langle q_i|$$

Removing the ill defined term of *U*

Introducing the term that we practically use

After acting on the Dyson series of *U*, one finds:

$$\hat{\mathcal{P}}(0,-\infty)\,|q\rangle = \left(\hat{\mathbf{1}} - \int |q_j g\rangle \lim_{\epsilon\to 0} \frac{\langle q_j g|\,\hat{H}\,|q_i\rangle}{E_{q_j g} - E_{q_i} - i\epsilon} \langle q_i|\right.$$

$$\left. -\frac{1}{2}\int |q_f\rangle \lim_{\epsilon\to 0} \frac{\langle q_f|\,\hat{H}\,|q_j g\rangle}{(E_{q_j g} - E_{q_f} + i\epsilon)} \lim_{\epsilon\to 0} \frac{\langle q_j g|\,\hat{H}\,|q_i\rangle}{(E_{q_j g} - E_{q_i} - i\epsilon)} \langle q_i| \right) |q\rangle$$

Order g term unaffected

The structure remains valid under q→ qq

- *This is the very same familiar expression we practically use after introducing the wave-function normalization **Z**, but this time from first principles!*

The WF for quark anti-quark

Assuming (wrongly) that normalization is conducted via $|q\bar{q}\rangle \longrightarrow \sqrt{Z_q}\sqrt{Z_{\bar{q}}}\,|q\bar{q}\rangle$,
at g^2, the general structure of the WF for two partons based on *U* contains “self energy” and “gluon exchange” contributions:

$$|q\bar{q}\rangle_{g^2} = \int ((s.e.) + (branch - cut)\,|q\bar{q}\rangle$$

The “gluon exchange” contribution is associated with a “branch cut integral”:

$$I = \int \frac{d^d\boldsymbol{p}}{(2\pi)^d} \lim_{\epsilon\to 0} \frac{\boldsymbol{p}}{\beta\boldsymbol{p}^2 - i\epsilon} \cdot \lim_{\epsilon\to 0} \frac{\boldsymbol{p}-\alpha\boldsymbol{k}}{\beta\boldsymbol{p}^2 - \gamma\left(\boldsymbol{p}-\alpha\boldsymbol{k}\right)^2 - 2i\epsilon}$$

- Based on *P,* the structure will consists of “self-energy”, “2 Weizsäcker-Williams fields” and *anti-Hermitian combination* (due to the commutator) of “branch-cut” contributions:

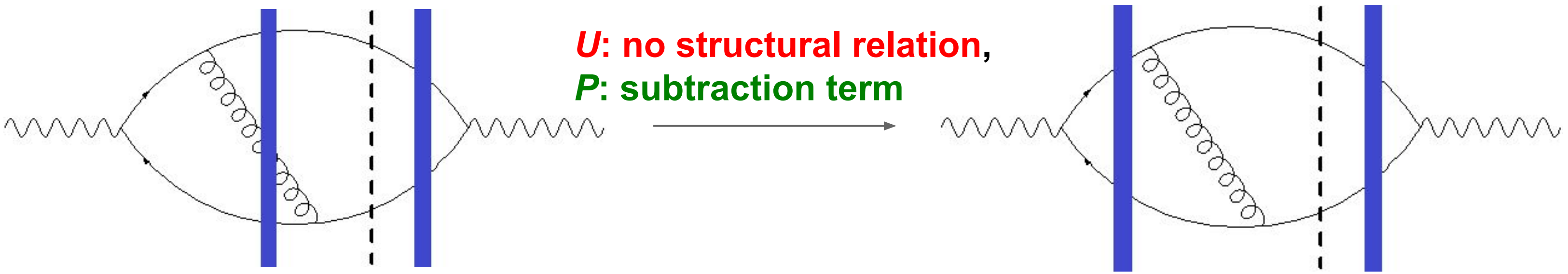
$$|q\bar{q}\rangle_{g^2} = \int \left((s.e.) + (2w.w.) + (branch - cut) - (branch - cut)^\dagger\right)|q\bar{q}\rangle$$

The “gluon exchange” contribution is associated with the 2 WW fields:

$$I = \int \frac{d^d\boldsymbol{p}}{(2\pi)^d} \lim_{\epsilon\to 0} \frac{\boldsymbol{p}}{\beta\boldsymbol{p}^2 - i\epsilon} \cdot \lim_{\epsilon\to 0} \frac{\boldsymbol{p}-\alpha\boldsymbol{k}}{\gamma\left(\boldsymbol{p}-\alpha\boldsymbol{k}\right)^2 + i\epsilon}$$

NLO cross sections: *U* vs *P*

The crucial (unbridgeable) difference between *U* and *P* emerges when computing the gluon exchange with shockwave prior to the gluon emission.



- ***Based on U***: leads to extremely complicated integrals which contain a measure-0 of unregularizable delta-functions. See appendix J in "*Dijet impact factor in DIS at next-to-leading order in the Color Glass Condensate*", F. Salazar.

- ***Based on P***: trivial calculation (subtraction term):

$$\frac{d\sigma_{V\,ex.}}{dk_1^+\,d^2k_1\,dk_2^+\,d^2k_2} = -\frac{2\alpha_{em}\,\alpha_s\,N_c}{(2\pi)^6 q^+}\left(\sum e_f^2\right)\delta(q^+ - k_1^+ - k_2^+)$$
$$\times \int_{\overline{x},\overline{y},x',y',z}\int_0^{1-\vartheta} d\xi\; e^{-ik_1\cdot(x'-\overline{x})-ik_2\cdot(y'-\overline{y})}\left((2\vartheta-1)(2\vartheta+2\xi-1)+1\right)\frac{4\vartheta(1-\vartheta-\xi)+2\xi}{\xi\vartheta(1-\vartheta)}$$
$$\times \frac{R'\cdot\overline{R}}{|R'|\,|\overline{R}|}\frac{X\cdot Y}{X^2\,Y^2}\,\tilde{Q}\bar{Q}\,K_1\left(\tilde{Q}|R'|\right)K_1\left(\bar{Q}|\overline{R}|\right)\mathcal{W}\left(x',\,y',\,\overline{y},\,\overline{x}\right).$$

Analytic properties of perturbative calculations

- **For U, non-intuitive properties appears:**

1) *The cross section can turn very large and negative.*
2) *The result involve contributions which are not Fourier transformable.*
3) *The NLO is bigger than LO and so on.*
4) *JIMWLK cannot be shown at the amplitude level.*

- **For P:**

None of these problems.

***Positive definite energy denominator with Intuitive properties*.**

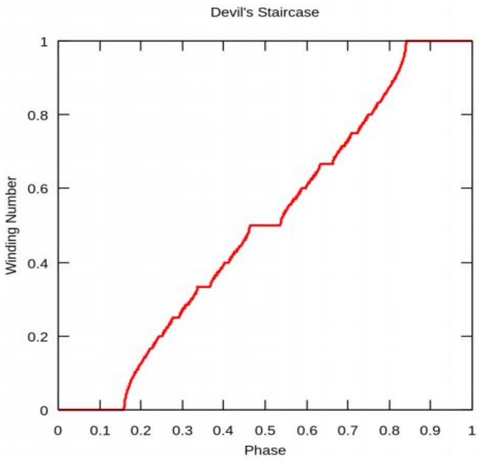
- **Occam's razor:** “*Entities must not be multiplied beyond necessity*”.

Singular Functions

1) *f(x)* is continuous (but not absolutely continuous), and non-constant on [a, b].

2) There exists a set N of measure 0 such that for all x outside of N the derivative *f'(x)* exists and is zero, that is, the derivative of *f(x)* vanishes almost everywhere.

A standard example of a singular function is the *Cantor ternary function* (or alternatively as *Lebesgue's singular function* or *Devil's staircase*). In practical terms, a singular function can be expressed as a **continuous sum of delta functions**.



Theoretical implications

"By their fruits ye shall know them" (*Matthew 7:16*)

- **Optical theorem for U**:

$$\hat{U}^\dagger(t,\, t_0)\, \hat{U}(t,\, t_0) \;=\; (\hat{\mathbf{1}} - i\hat{T}^\dagger)\, (\hat{\mathbf{1}} + i\hat{T}) \;=\; \hat{\mathbf{1}}$$

$$i(\hat{T} - \hat{T}^\dagger) = -\hat{T}^\dagger \hat{T}$$

Implications: *Froissart bound*, *Pomeranchuk bound*.

- **No optical theorem for P**:

$$\hat{\mathcal{P}}(t,\, t_0) \equiv \sqrt{(\hat{\mathbf{1}} - i\hat{T}^\dagger)^{-1}\, (\hat{\mathbf{1}} + i\hat{T})^{-1}}\, (\hat{\mathbf{1}} + i\hat{T})$$

$$\hat{\mathcal{P}}^\dagger(t,\, t_0)\, \hat{\mathcal{P}}(t,\, t_0) \;=\; (\hat{\mathbf{1}} - i\hat{T}^\dagger)\, (\hat{\mathbf{1}} - i\hat{T}^\dagger)^{-1}\, (\hat{\mathbf{1}} + i\hat{T})^{-1}\, (\hat{\mathbf{1}} + i\hat{T}) \;=\; \hat{\mathbf{1}}$$

- **Cutkoski**: "*If a certain number of propagators go on-shell at a singularity, then the discontinuity in the amplitude from the corresponding branch cut is computed by replacing* $\frac{i}{k^2 - m^2 - i\epsilon} \longrightarrow \delta(k^2 - m^2)$". However, discontinuities are ***not predicted*** by the Schrodinger equation. Using P: $\lim_{\epsilon \to 0} \mathcal{M}\,(s - i\epsilon) \;=\; \lim_{\epsilon \to 0} \mathcal{M}\,(s + i\epsilon)$

For those who criticise

- Please ask yourself the following questions:

1) ***On what basis do you iterate limits freely?***

2) ***How does the "WF normalization" or "LSZ Z" get its value at finite times?***

3) ***Which operator transforms the original expression for the quark WF (based on U) to the expansion that we work with in practice?***

Summary

1) The unitarity of the Dyson series is preserved for functions, but is broken by distributions.

2) The discrete part of the dynamics is contained in the normalization operator N.

3) The solution P is manifestly unitary, even when the terms of the series are conditionally convergent, or distributions are used.

4) Wider class of quantum field theories, in which unitarity is known to be broken, can now studied normally.

5) *Happy end for the "saga"*: the elegant structure have appeared again.