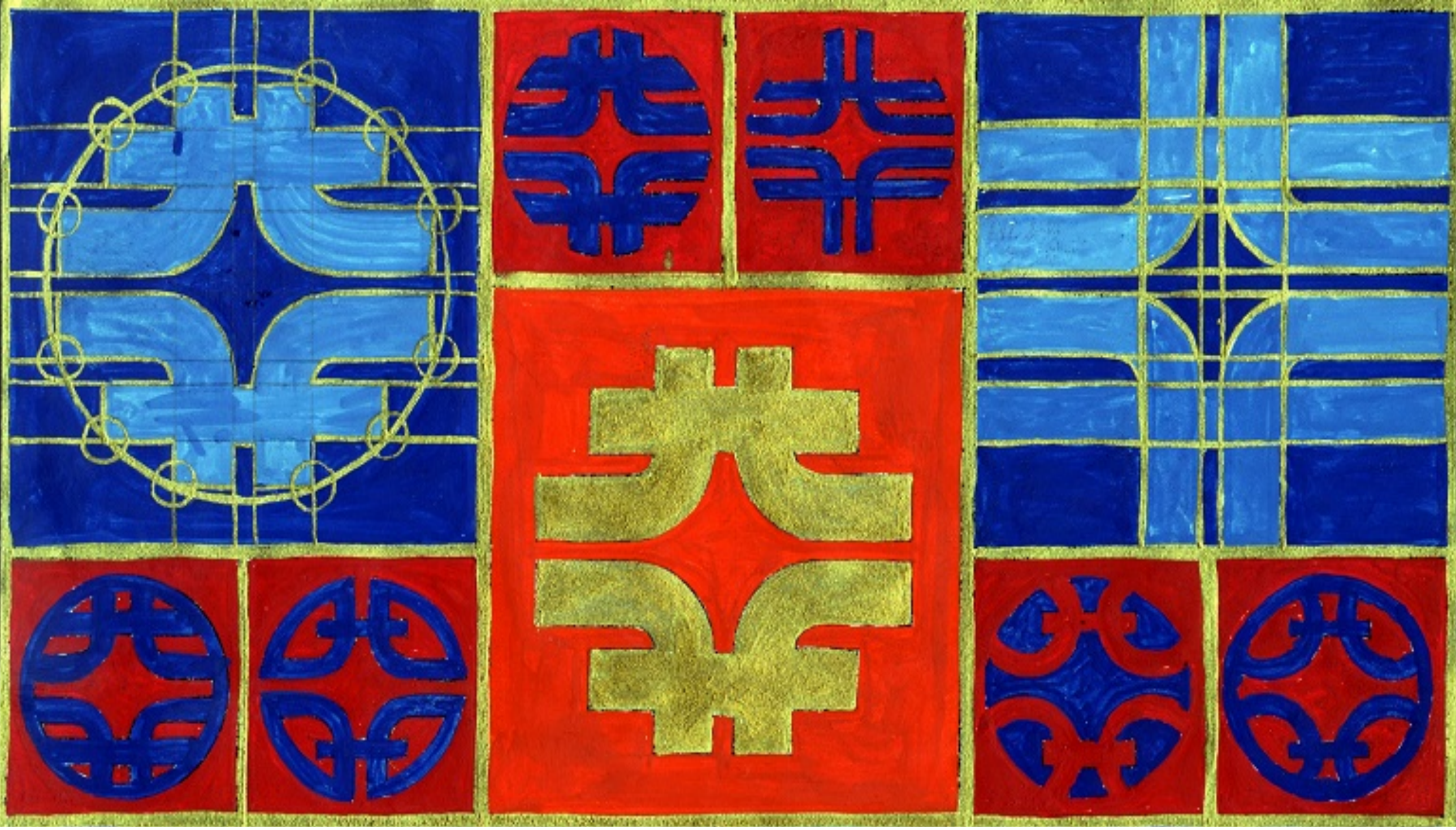


Lattice QCD for Neutrinos

William I. Jay (Fermilab)

Fermilab Neutrino Seminar Series — 11/1/2020

Goals of the talk:

- The importance of grounding neutrino-nucleus scattering experiments in QCD
- How to do this, schematically
- Some frontier calculations in lattice QCD over next 5-10 years, which I think are interesting

- Some things this talk is ***not:***
  - A comprehensive review of the state of the art in LQCD for neutrino-nucleus scattering
  - A seminar about recent results from lattice QCD

Useful references

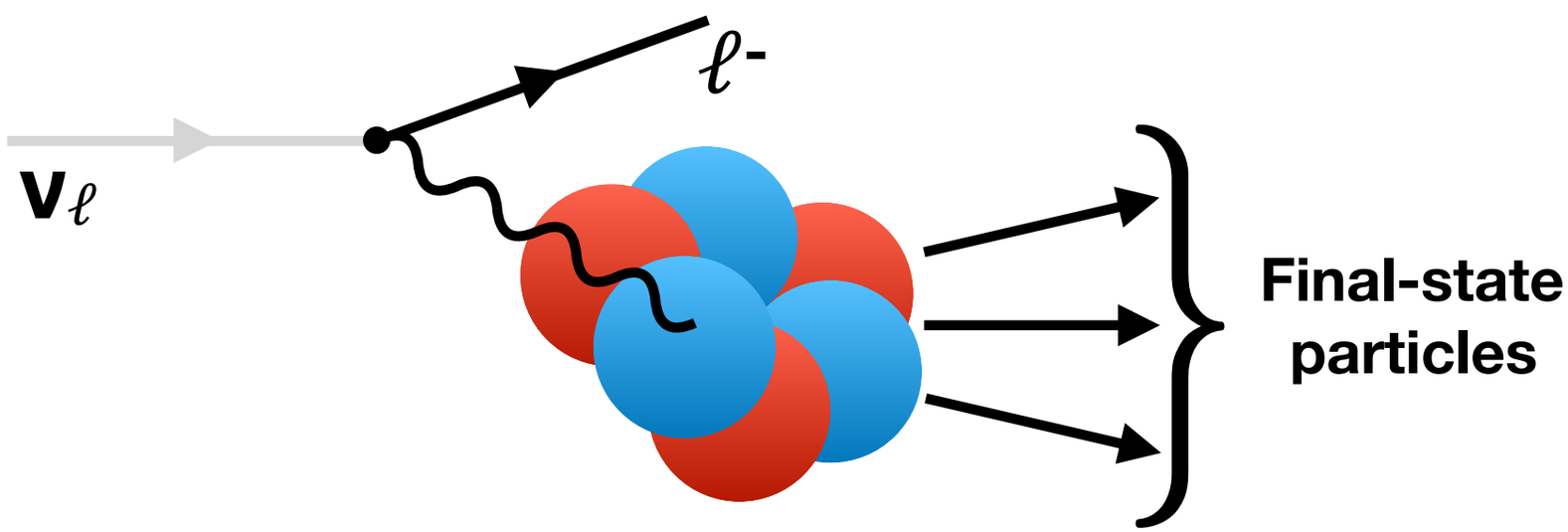
- USQCD white paper [Lattice QCD and Neutrino-Nucleus Scattering]
- 3 x Snowmass Letters of Interest:
  1. Wagman & Rocco [Connecting QCD to neutrino-nucleus scattering]
  2. Isaacson, Jay, Lovato, Machado, and Rocco [Event Generators for Accelerator-Based Neutrino Experiments]
  3. Lovato, Pastore, and Rocco [Microscopic approaches to neutrino-nucleus interactions]
- Flavour Lattice Averaging Group (FLAG) [2019 Review]
- Many useful review-level documents (Feel free to ask!)

Outline

1. Introduction / Motivation
2. Connections to QCD
3. Lattice QCD
4. Non-perturbative shallow inelastic scattering
   A. Backus-Gilbert Reconstruction
   B. Orthogonal Polynomial Reconstruction
5. Summary / Take-home Points

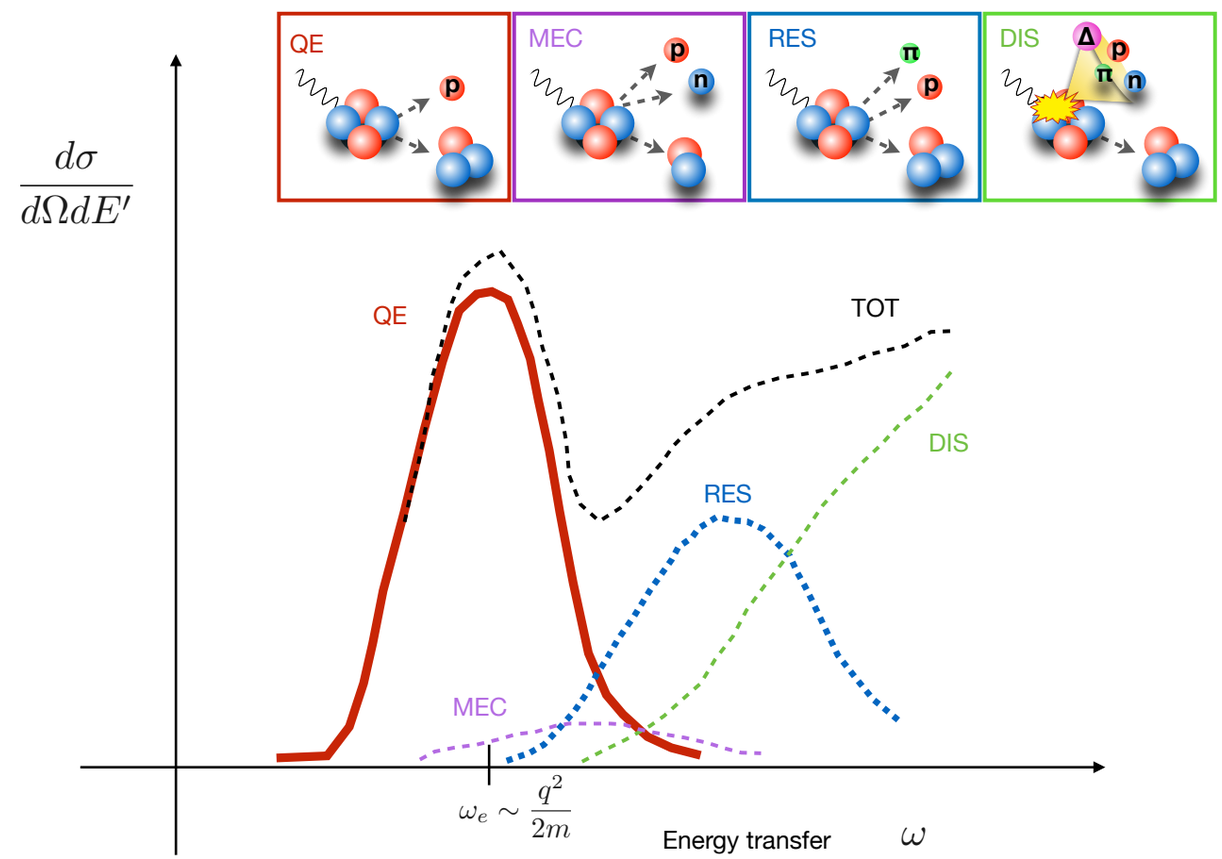
Motivation

- Neutrino experiments are really hard!
- Experimentally, neutrino energies are never measured directly. They are reconstructed from the measured final state.
- Typical target systems are large and complex: water, liquid scintillator, and liquid Argon



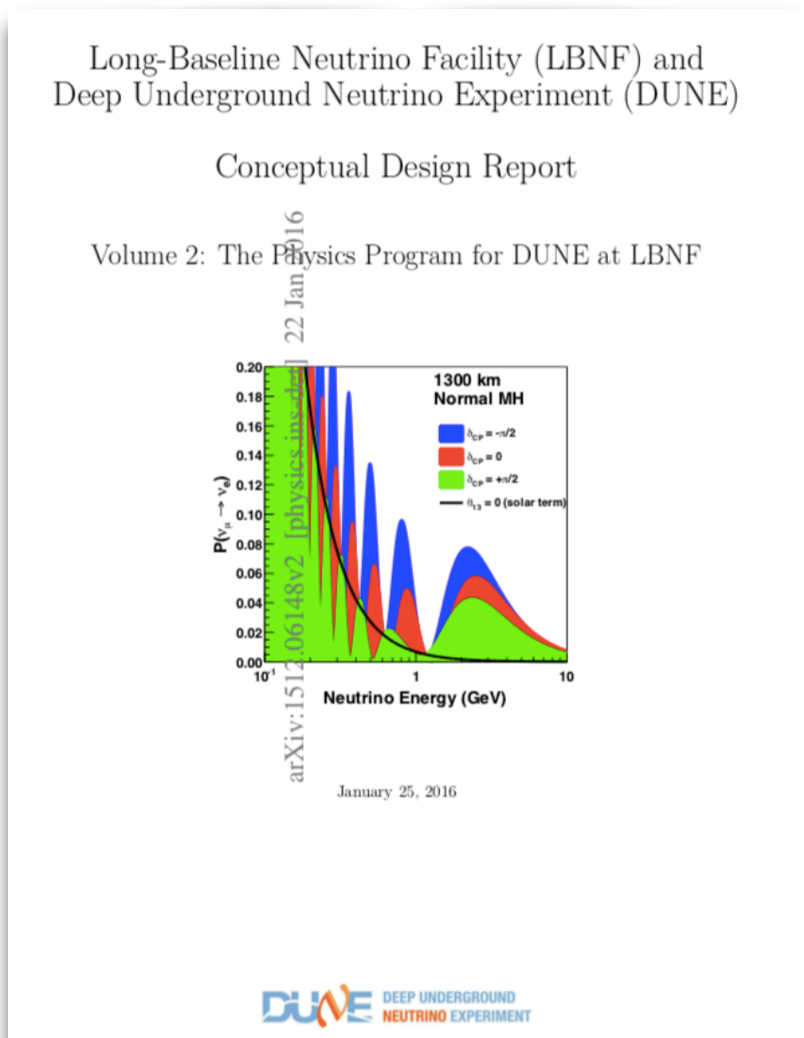
Motivation

- Neutrino-nucleus (ν-A) scattering is theoretically daunting
- Multi-scale, multi-process, many-body, non-perturbative problem
- DUNE and T2HK mark the beginning of the “precision era" of neutrino physics



Motivation

- High-precision experiments require commensurate high-precision theory


Long-Baseline Neutrino Facility (LBNF) and
Deep Underground Neutrino Experiment (DUNE)

Conceptual Design Report

Volume 2: The Physics Program for DUNE at LBNF

arXiv:1512.06148v2 [physics.ins-det] 22 Jan 2016

January 25, 2016

DEEP UNDERGROUND NEUTRINO EXPERIMENT

"Uncertainties exceeding 1% for signal and 5% for backgrounds may result in substantial degradation of the sensitivity to CP violation and the mass hierarchy."

Motivation

- High-precision experiments require commensurate high-precision theory
- To date, neutrino oscillations are the only beyond the Standard Model (BSM) physics processes observed in Earth-based experiments
- Neutrino systems are natural candidates for looking for other BSM signals
- Going beyond the Standard Model requires precise understanding the Standard Model
- Theoretical analyses must be quantitively grounded in the Standard Model: this means QCD!

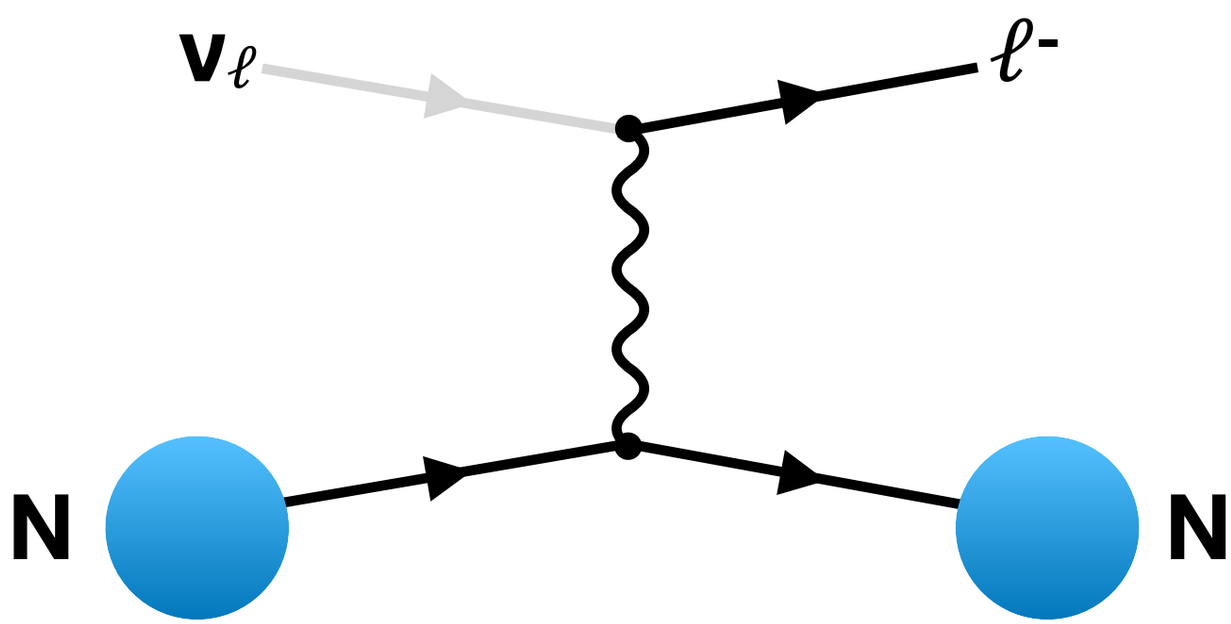
Event generation

- *Initial hard scattering*: neutrino kicks a nucleon
- *Intranuclear cascade*: the struck nucleon transfers energy to the rest of the nuclear system, which evolves to to produce the hadronic final state

Connections to QCD

Connections to QCD

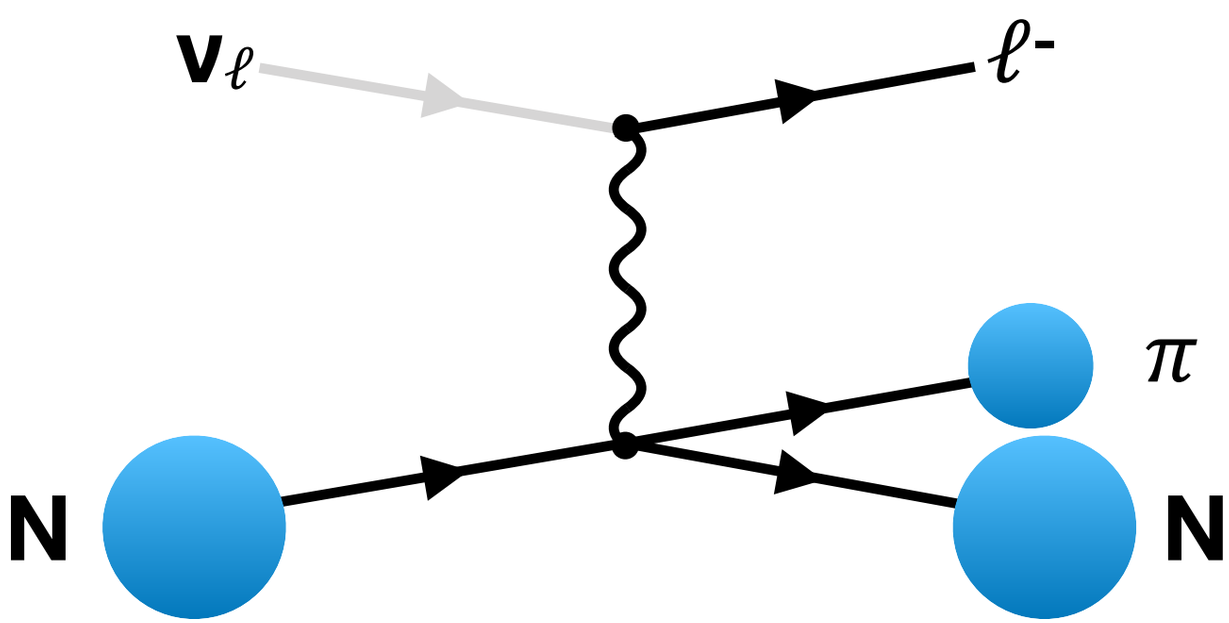
- Initial hard scattering process:
  - Low energy: ***elastic scattering***
  - Need QCD form factor: $\langle N|J(p)|N\rangle$
  - Reduces to nucleon "charges" when |**p**|→0



Connections to QCD

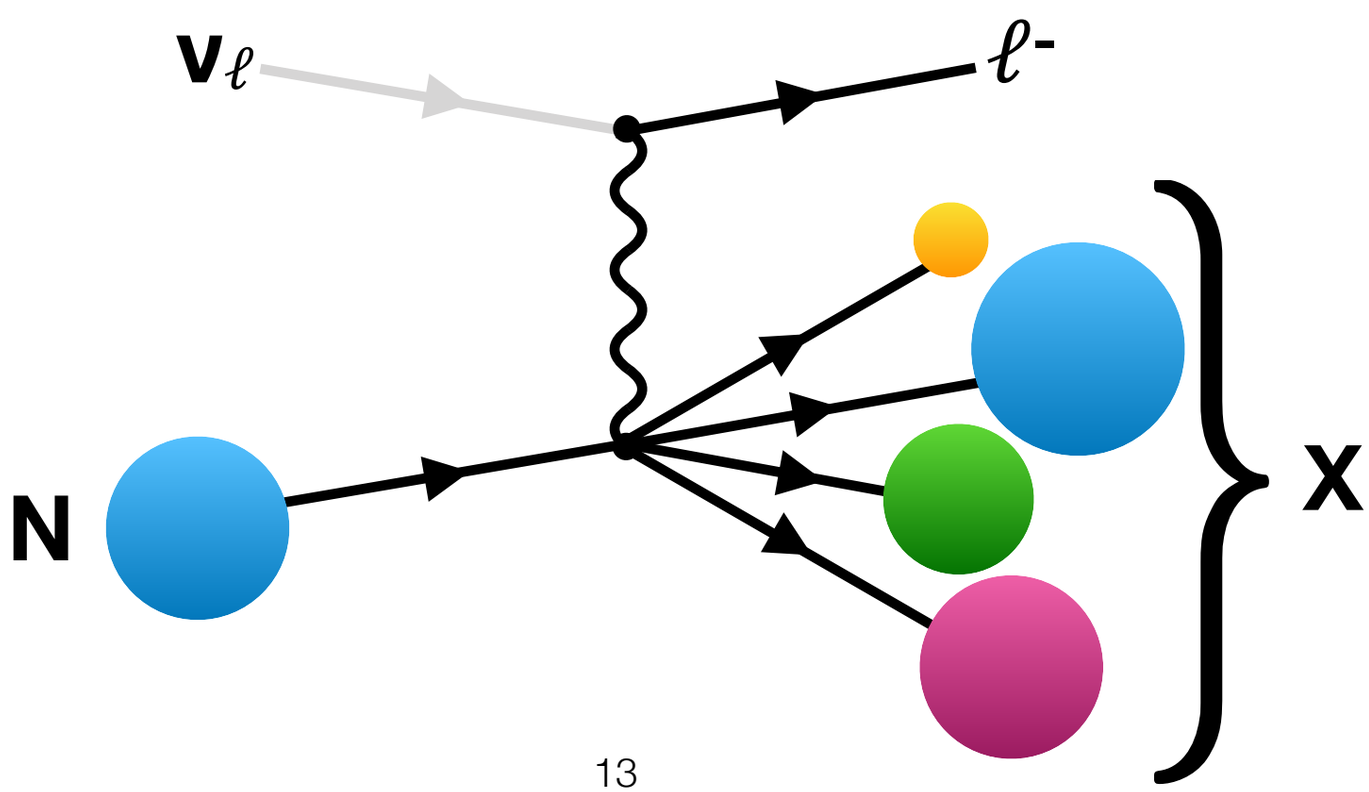
- Initial hard scattering process:
  - Intermediate energy: ***inelastic scattering***
  - Need amplitudes: $\langle N|J(p)|N\pi\rangle$

$$\langle N|J(p)|\text{few hadrons}\rangle$$



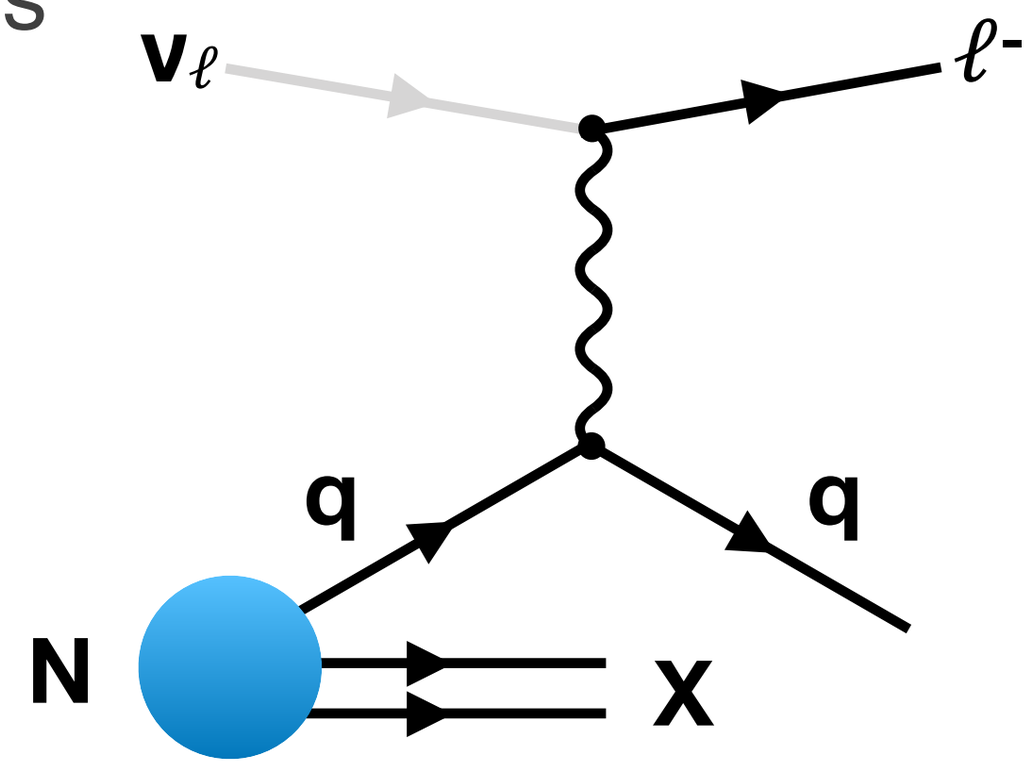
Connections to QCD

- Initial hard scattering process:
  - Intermediate energy: ***shallow inelastic scattering***
  - Many open channels: $\langle N | J(p) | X \rangle$
  - Energy too low to apply factorization safely



Connections to QCD

- Initial hard scattering process:
  - High energy: ***deep inelastic scattering***
  - Need: PDFs



$$\sigma(\text{hadron}) = \int \text{PDF} \times \sigma(\text{parton})$$

Connections to QCD

- Nuclear initial state: nuclear many-body theory
- Particle scattering and propagation during INC
- Nuclear Effective Theory:
- Dominant effects
  - 1-nucleon currents $\langle N|J|N\rangle$
  - 2-nucleon forces $|N(r_1)N(r_2)\rangle$
- Subdominant (but important)
  - 2-nucleon currents $\langle NN|J|NN\rangle$
  - 3-nucleon forces $|N(r_1)N(r_2)N(r_3)\rangle$

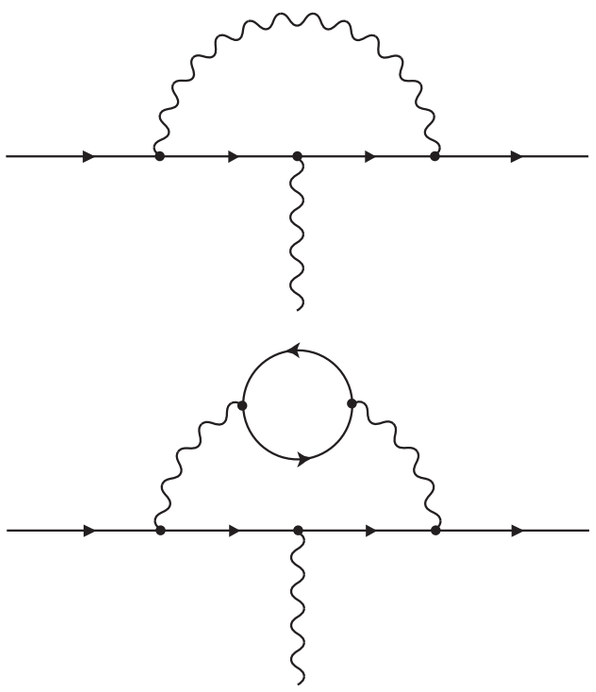
Lattice QCD

QCD as a QFT

- Quantum field theories ⟺ path integrals

$$\mathcal{Z} = \int \mathcal{D}[\text{fields}] e^{-iS[\text{fields}]}$$

- Weak coupling
  - ⟺ Particle-centric: particles interact weakly with quantum fluctuations
  - ⟺ Diagrammatic expansion
  - ⟺ S-matrix elements



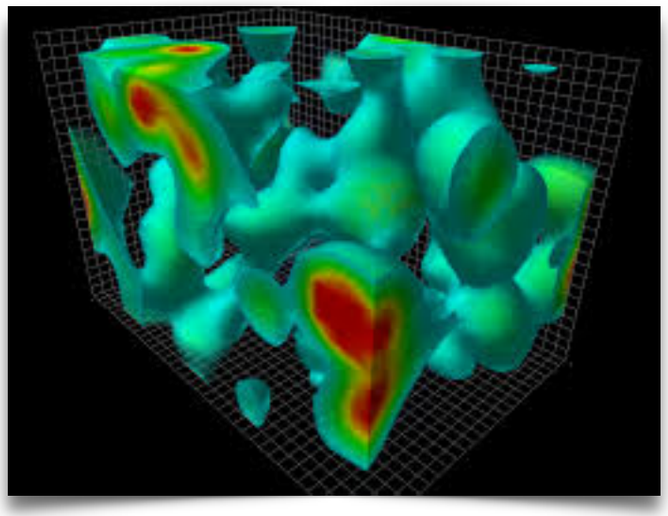
- Examples:
  - QED for (g-2)
  - QCD at high energies
  - Leptonic part of νA scattering

QCD as a QFT

- Quantum field theories ⟺ path integrals

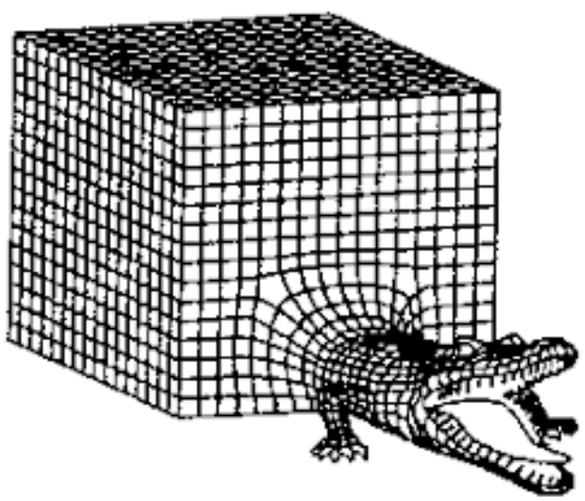
$$\mathcal{Z} = \int \mathcal{D}[\text{fields}] e^{-iS[\text{fields}]}$$

- Strong coupling
  - ⟺ Field-centric: particles emerge from correlated quantum fluctuations
  - ⟺ Need full path integral beyond perturbation theory
  - ⟺ Compute correlation functions
- Examples:
  - QCD at low energies
  - Hadronic part of νA scattering



Lattice QCD

$$\mathcal{Z} = \int \mathcal{D}[\text{fields}] e^{-iS[\text{fields}]}$$



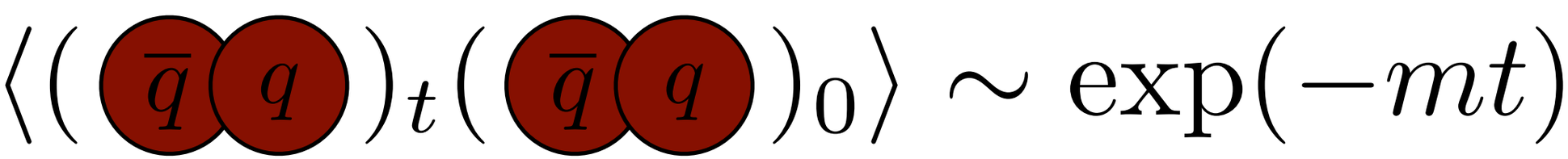
- Want: complete definition for the path integral
  1. Avoid UV divergences $\Longrightarrow$ use a finite lattice
  2. Avoid IR divergences $\Longrightarrow$ use a finite volume
  3. Avoid extreme cancellations $\Longrightarrow$ use Euclidean time
- $\mathcal{Z} \rightarrow$ Manifestly finite (but high-dimensional) sum
- Can evaluate numerically using Monte Carlo

Lattice QCD

- Lattice QCD is theoretical framework (not just code!)
- Some features and facts (both useful and annoying):
  - Generically, operators in a QFT couple to ***all*** states with matching quantum numbers
  - Quantum mechanics in a box: energy levels are discrete

Lattice QCD: particle masses

- 2-point correlation functions encode particle masses
- Analogy with condensed matter via: $\lambda = \dfrac{h}{mc}$
  - Correlation length $\lambda \longleftrightarrow$ Particle mass 1/m



Lattice QCD: particle masses

- Hadronic spectrum ⟷ QCD 2pt correlation functions

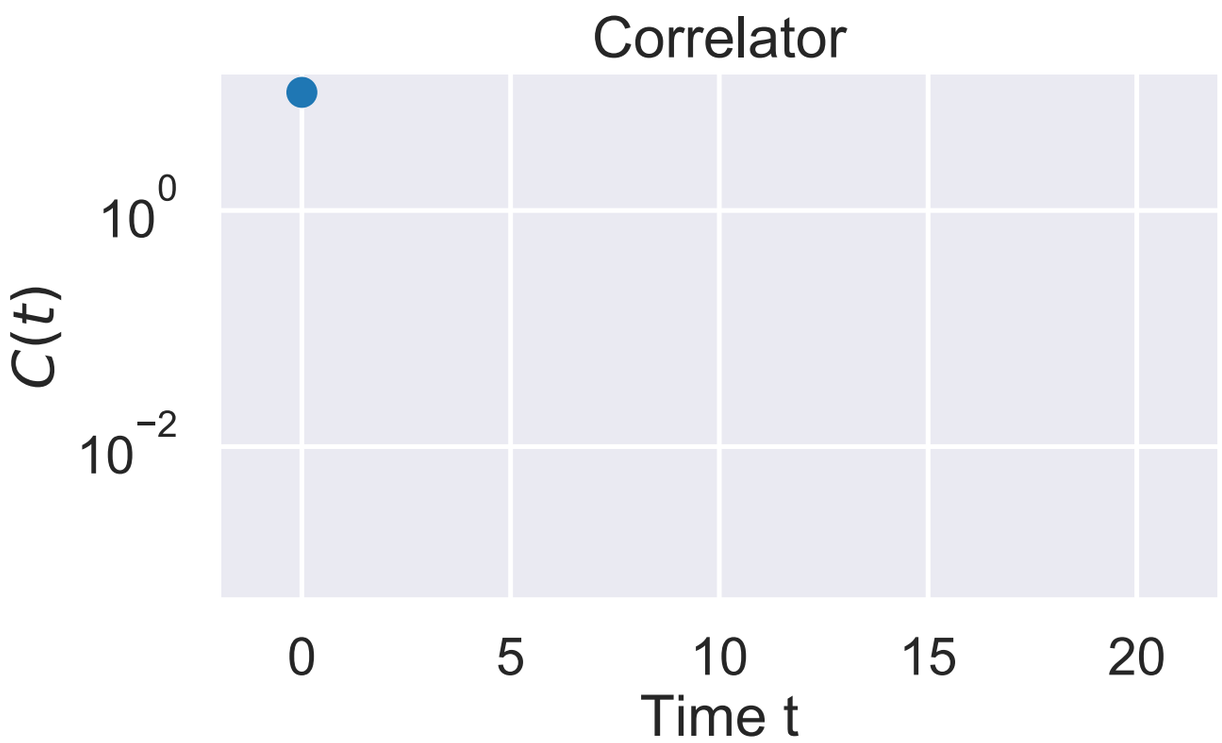
$$\begin{aligned}\langle O(t)O(0)\rangle &= \langle 0| e^{Ht}O(0)e^{-Ht}O(0)\,|0\rangle \\ &= \sum_n e^{-E_n t}\,\langle 0|\,O(0)\,|n\rangle\,\langle n|\,O(0)\,|0\rangle \\ &= \sum_n e^{-E_n t}\,|\langle 0|\,O(0)\,|n\rangle|^2 \\ &= \sum_n |Z_n|^2 e^{-E_n t}\end{aligned}$$

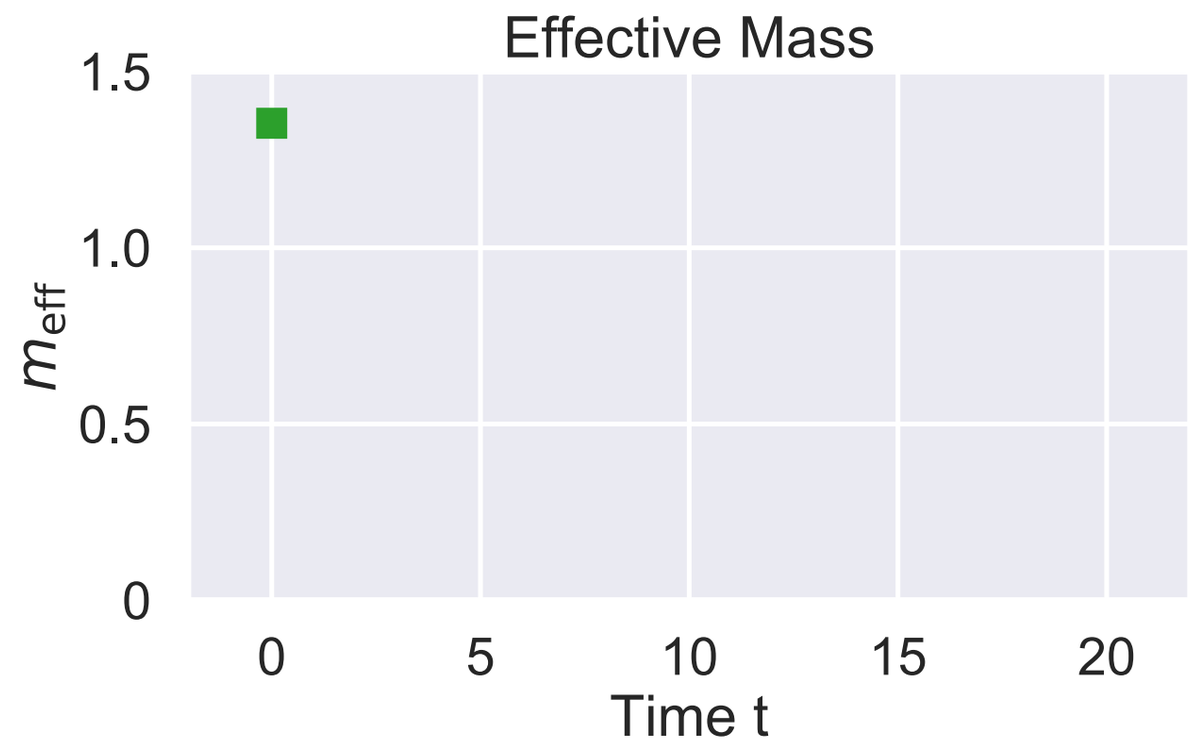
"The operators couple to an infinite tower of states."

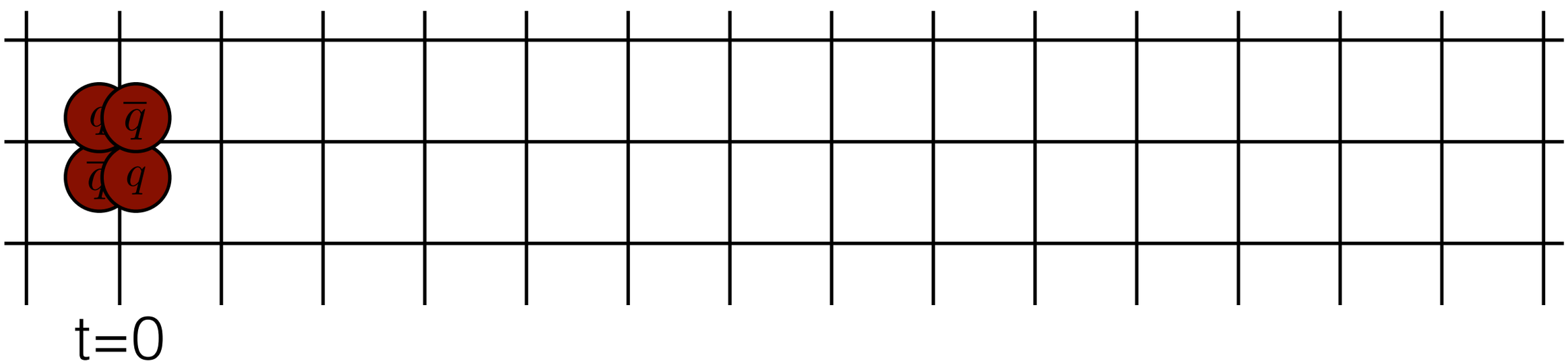
$$m_{\text{eff}} = \log\frac{C(t)}{C(t+1)} \overset{t\to\infty}{\sim} m_0$$

"The ground-state mass asymptotically dominates the Euclidean 2pt function."

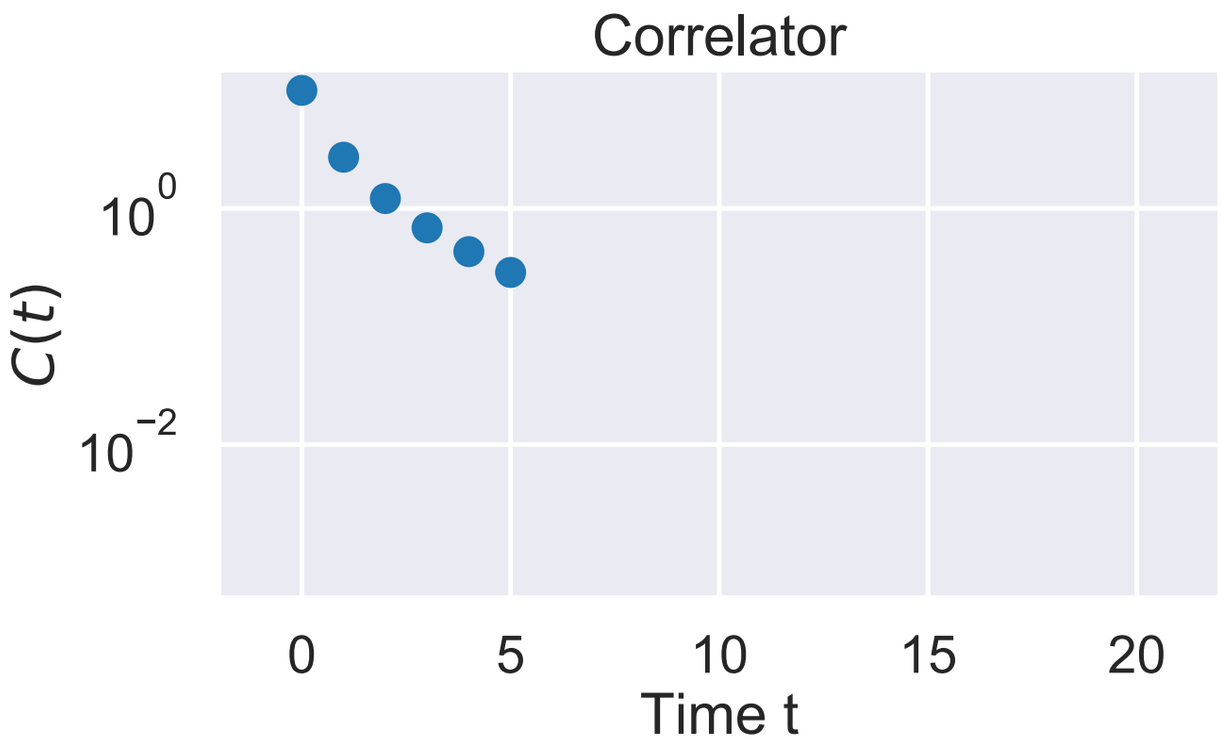
Lattice QCD: particle masses

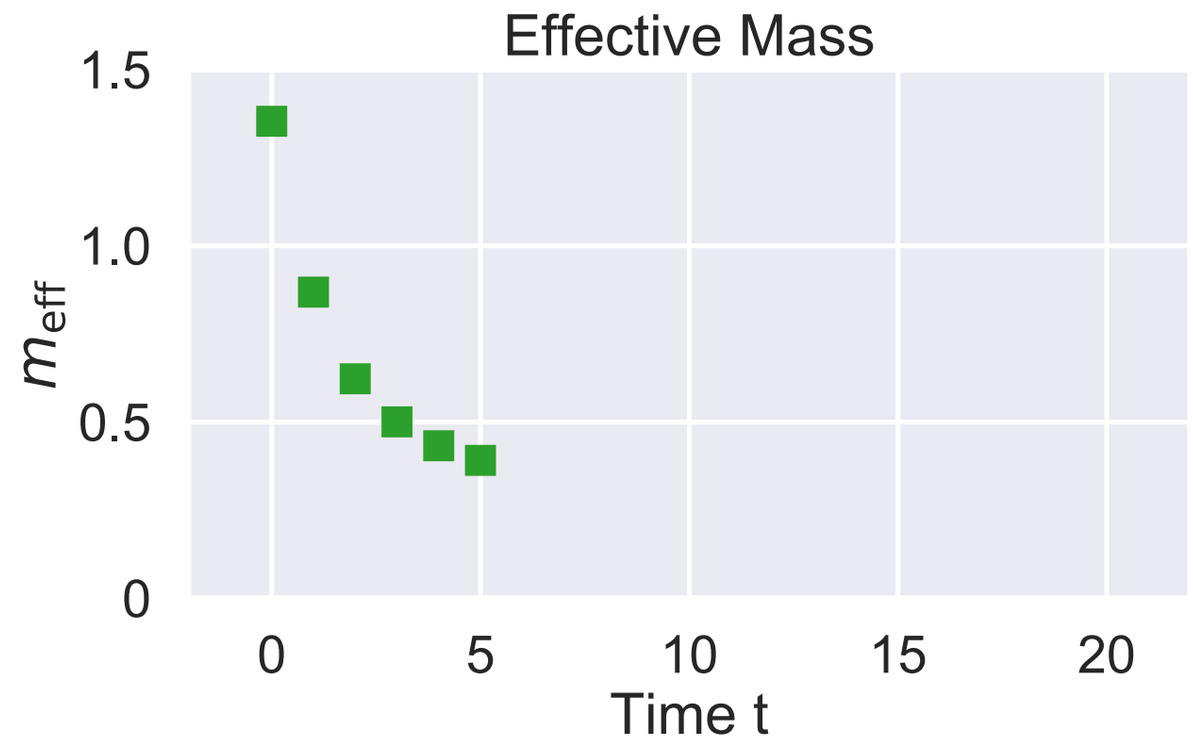


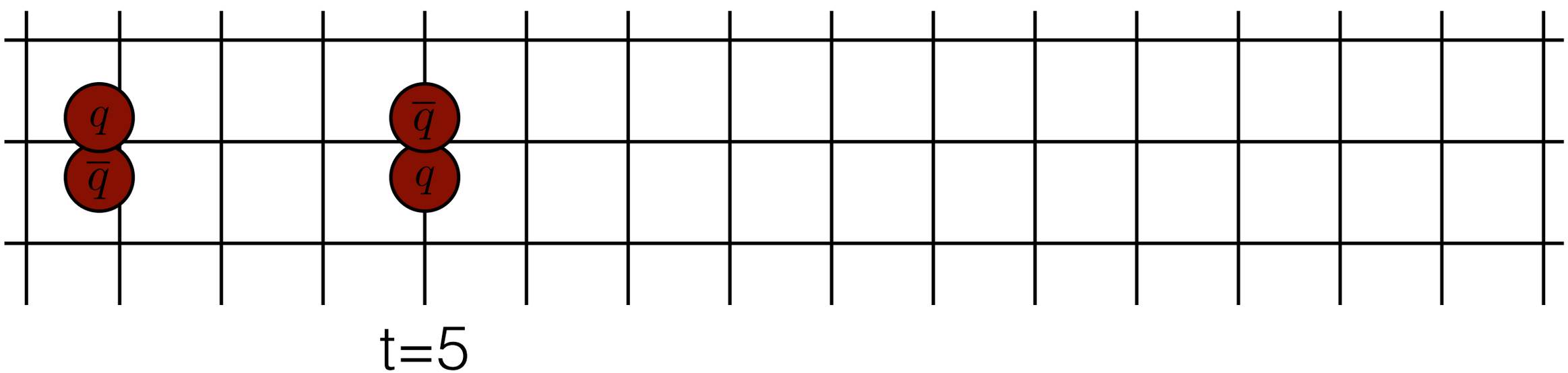




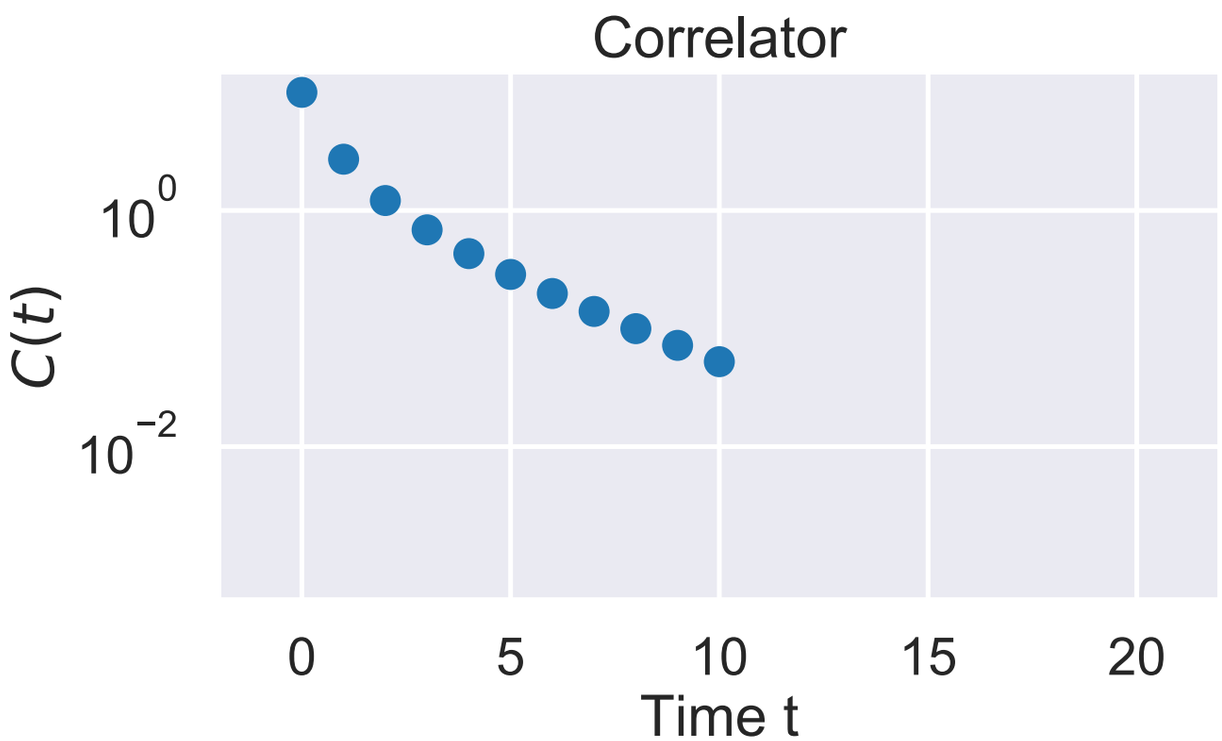
Lattice QCD: particle masses

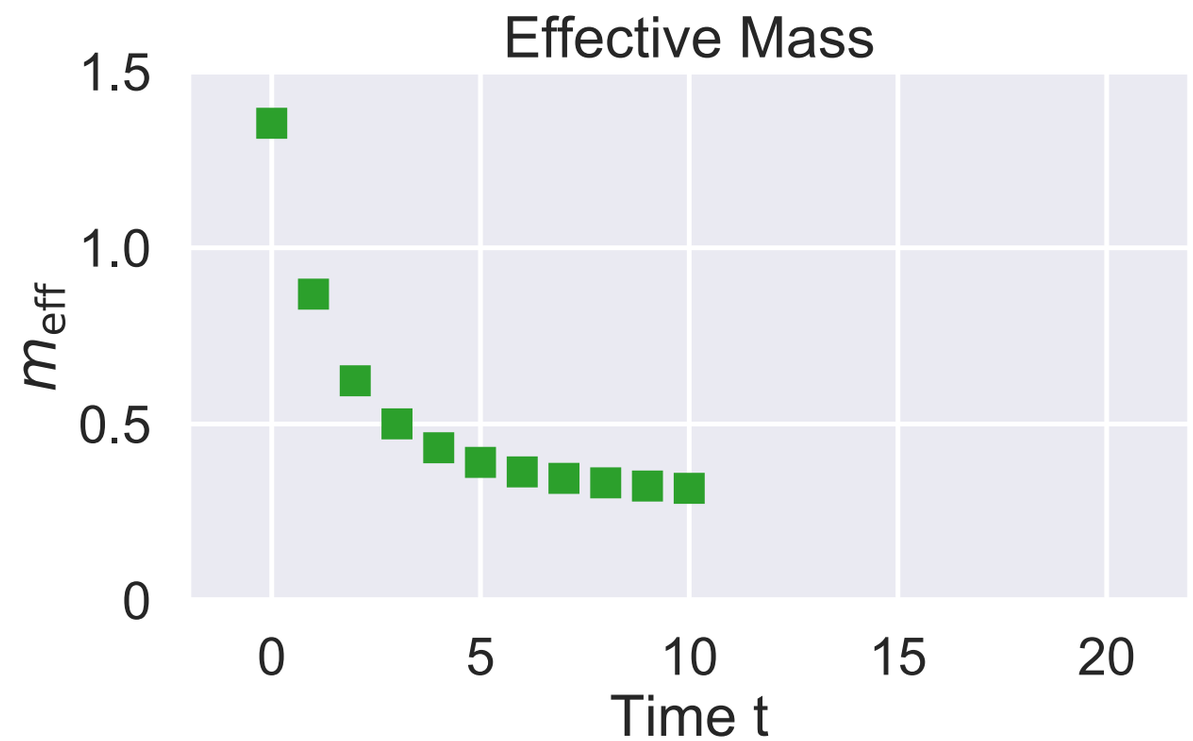


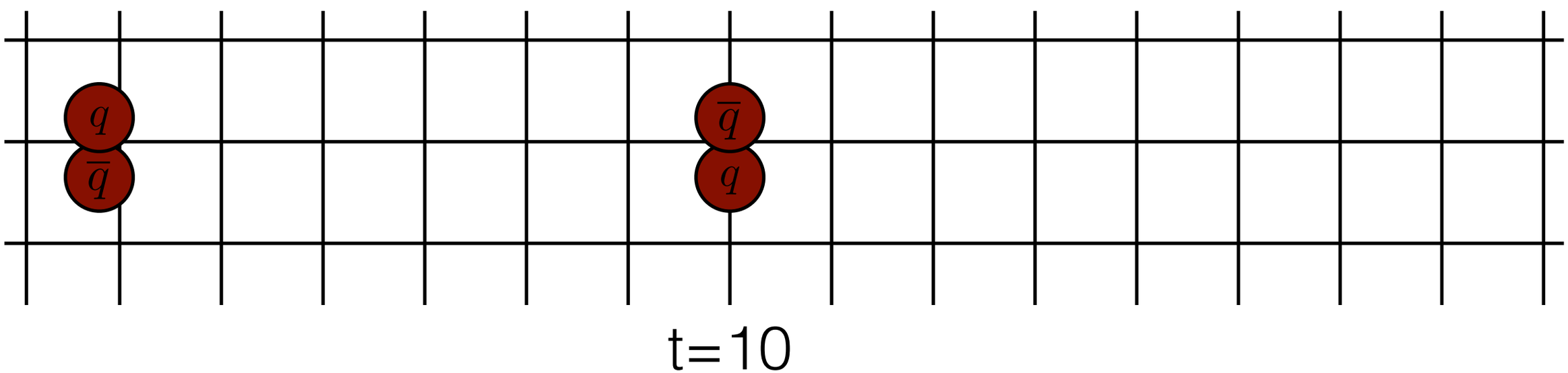




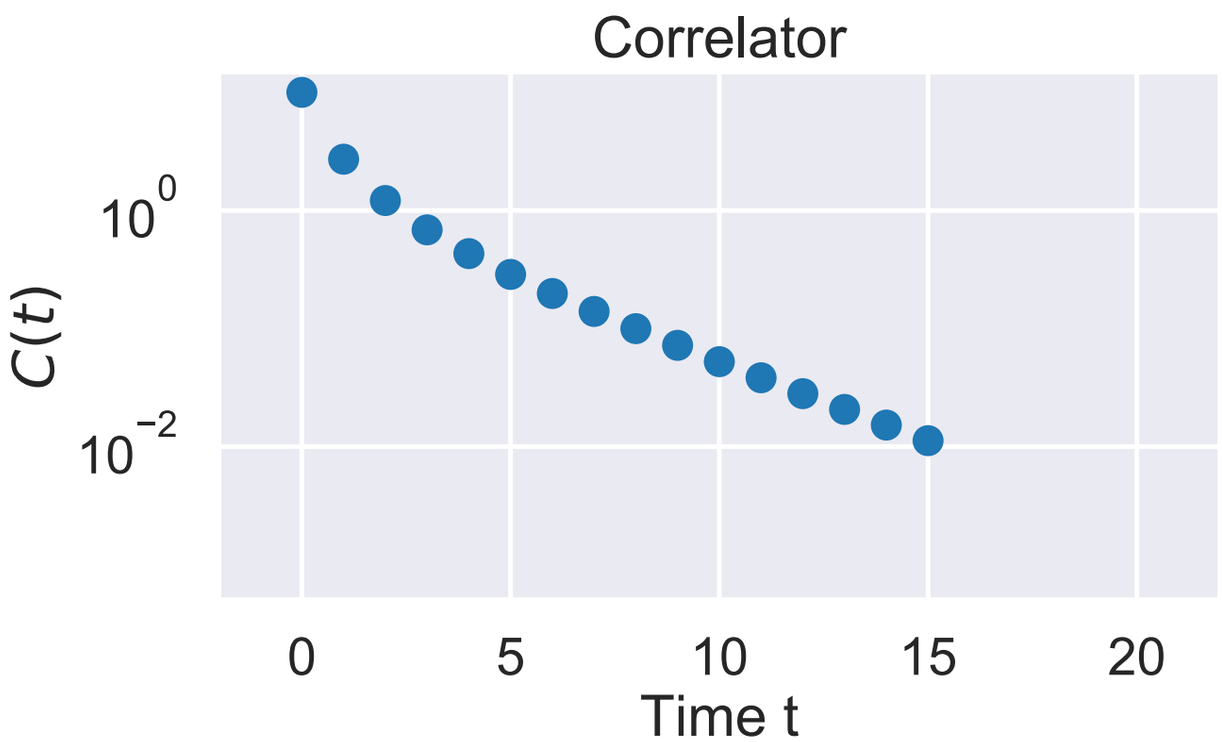
Lattice QCD: particle masses

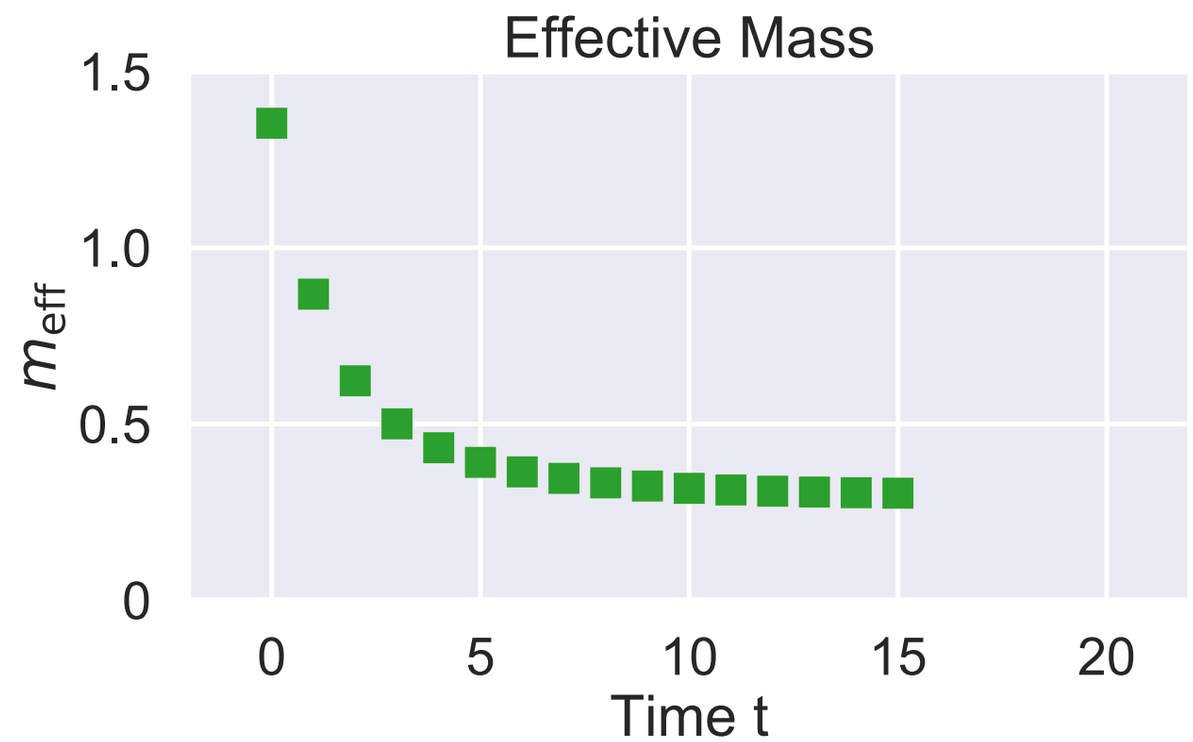


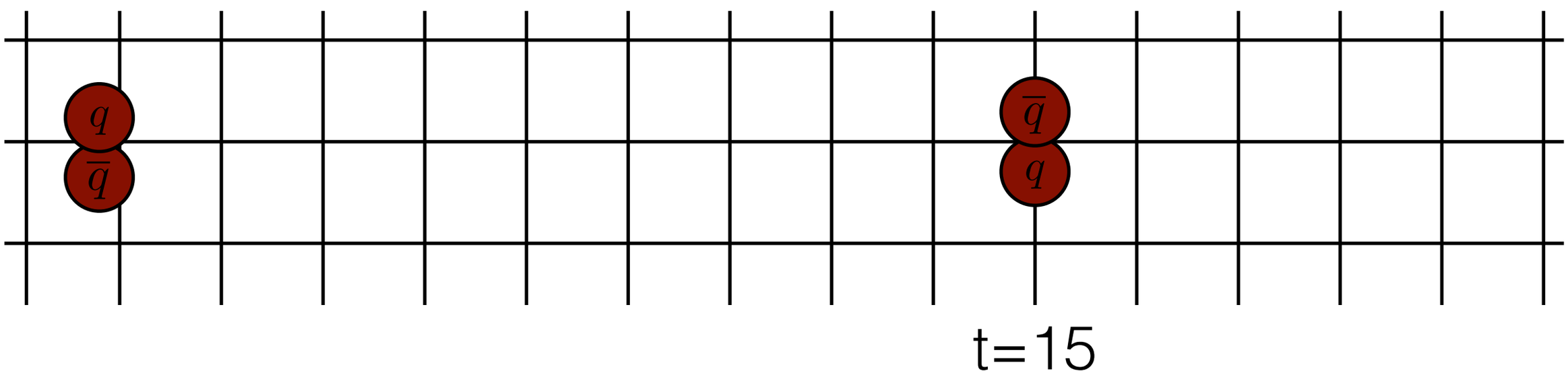




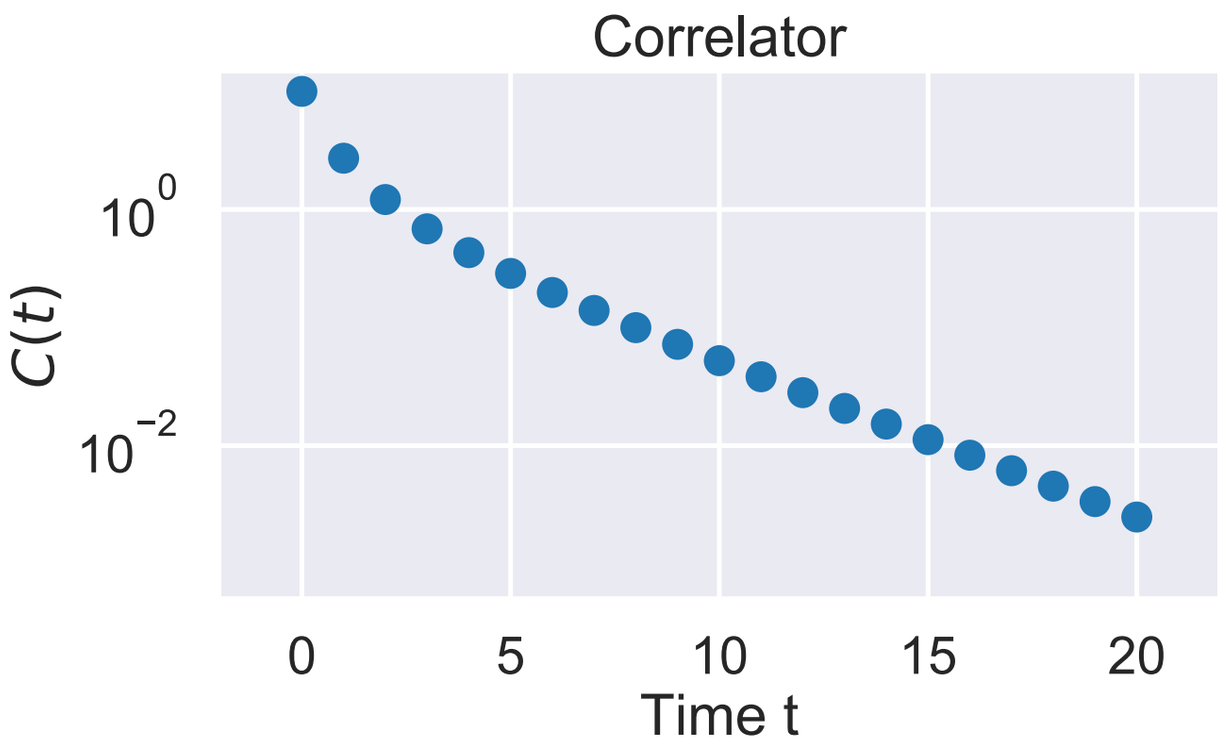
Lattice QCD: particle masses

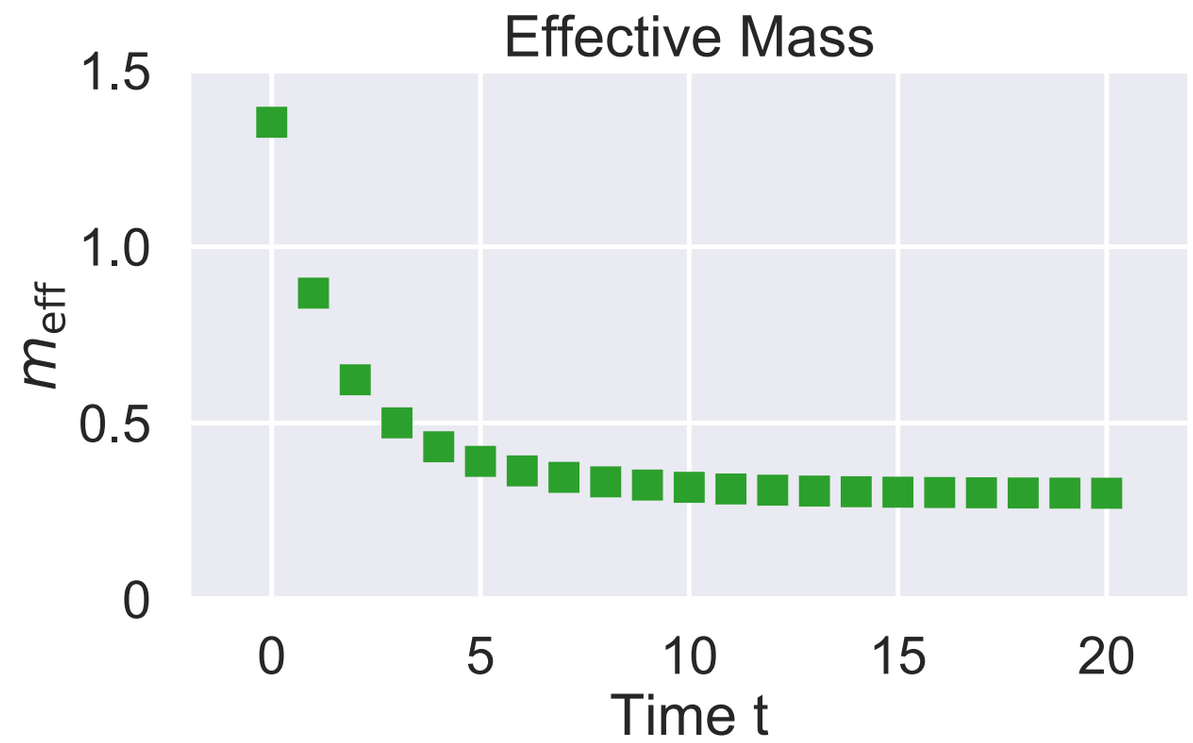


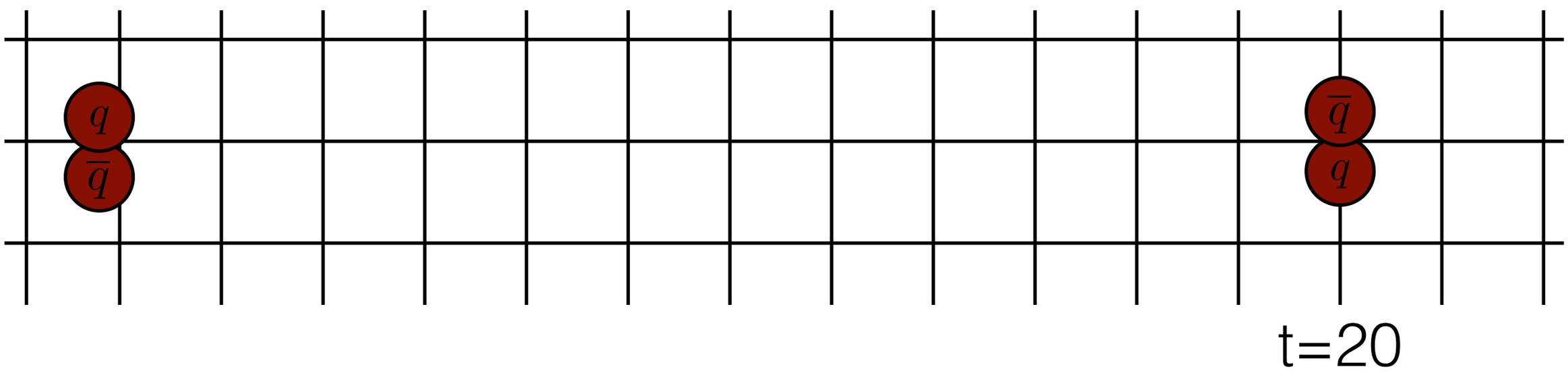




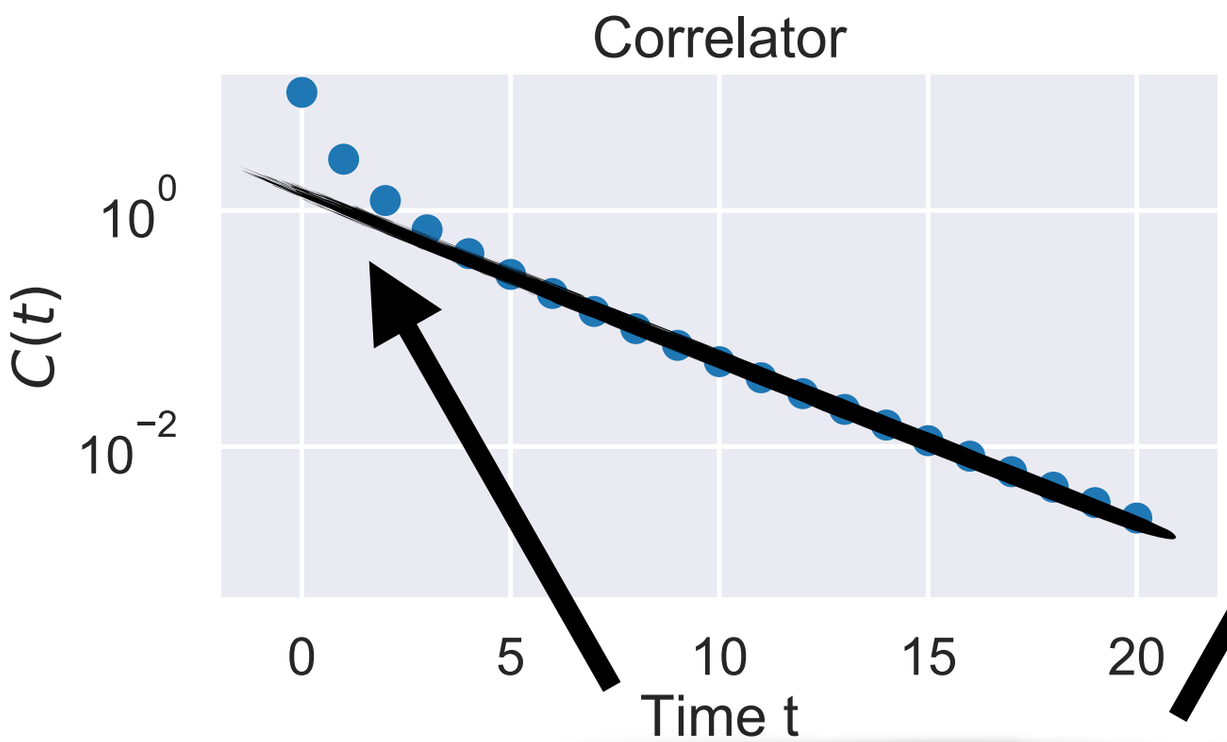
Lattice QCD: particle masses

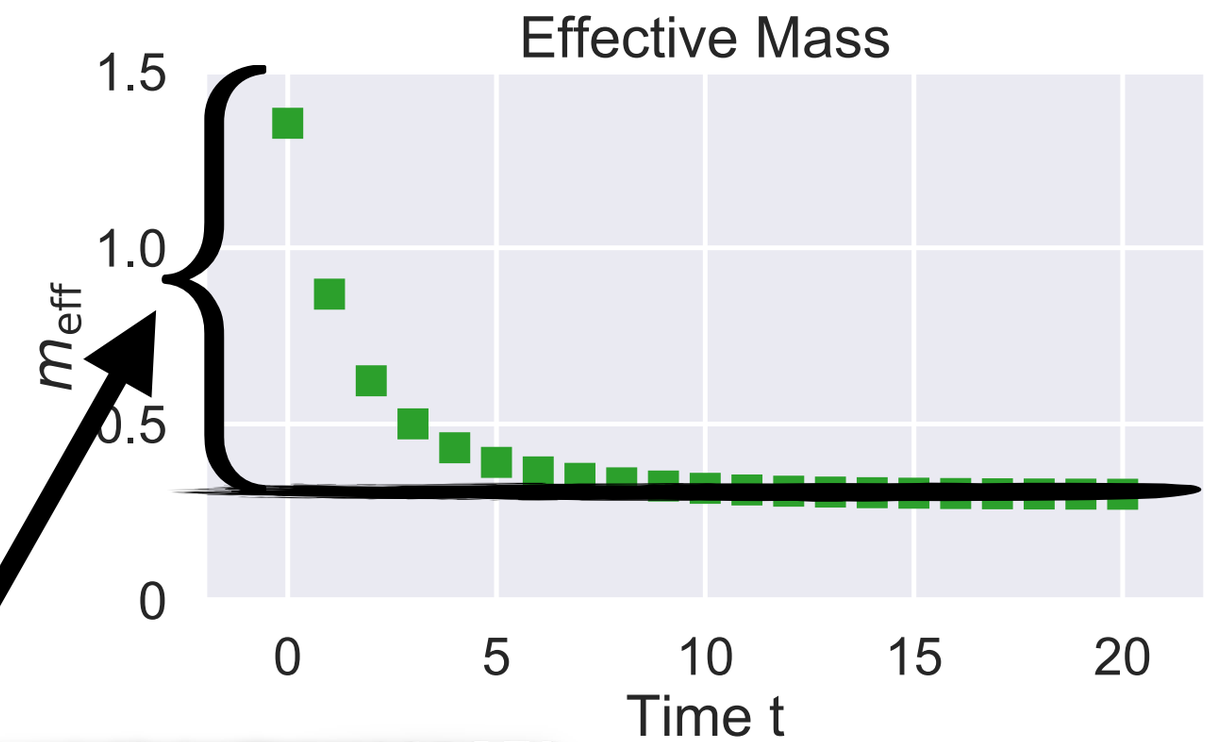




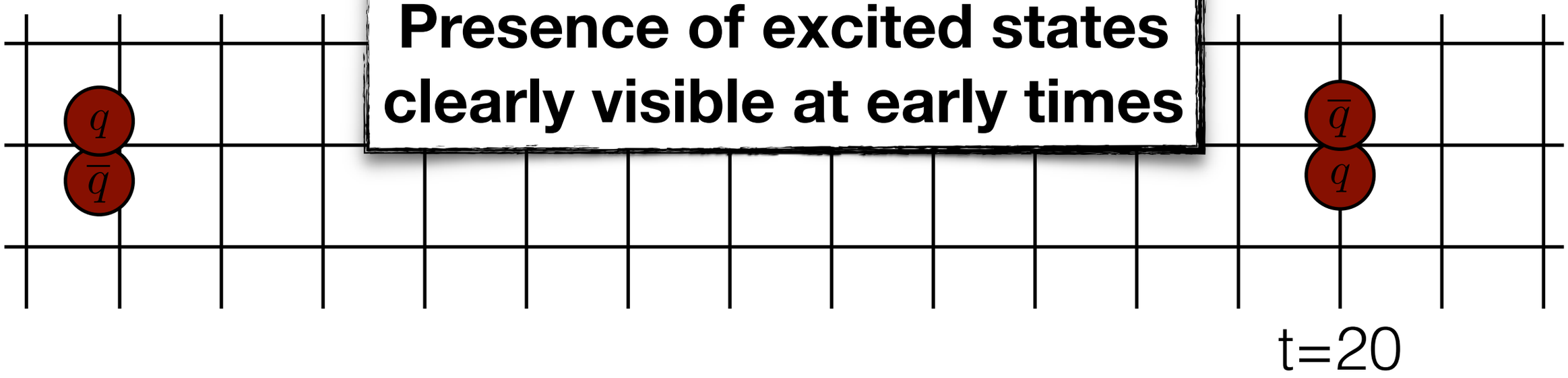


Lattice QCD: particle masses





Presence of excited states clearly visible at early times

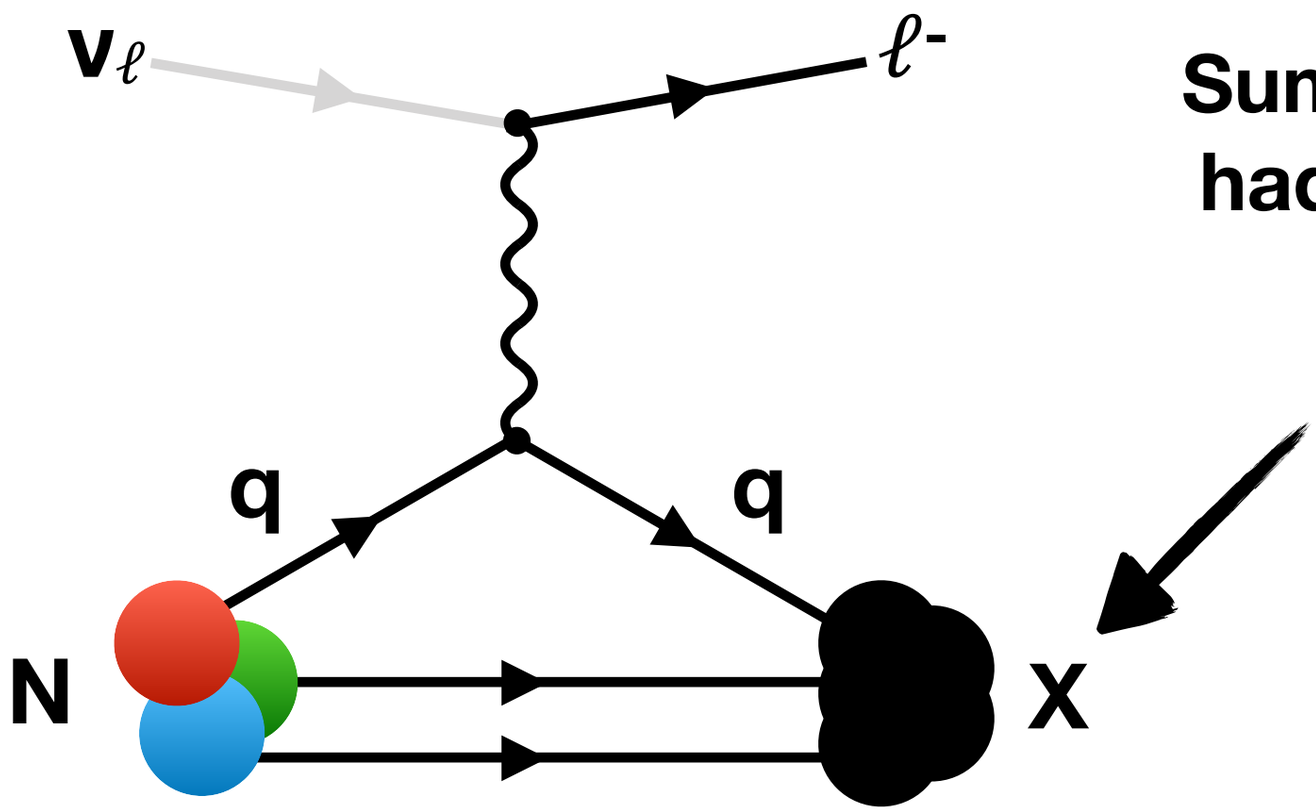


Lattice QCD: particle masses

- Operators couple to all possible excited states
- For spectroscopy, this fact is largely an annoyance
- However, the automatic presence of these states can be a tool as well
- Example: νN scattering with many open channels

Non-perturbative Shallow Inelastic Scattering

Shallow Inelastic Scattering

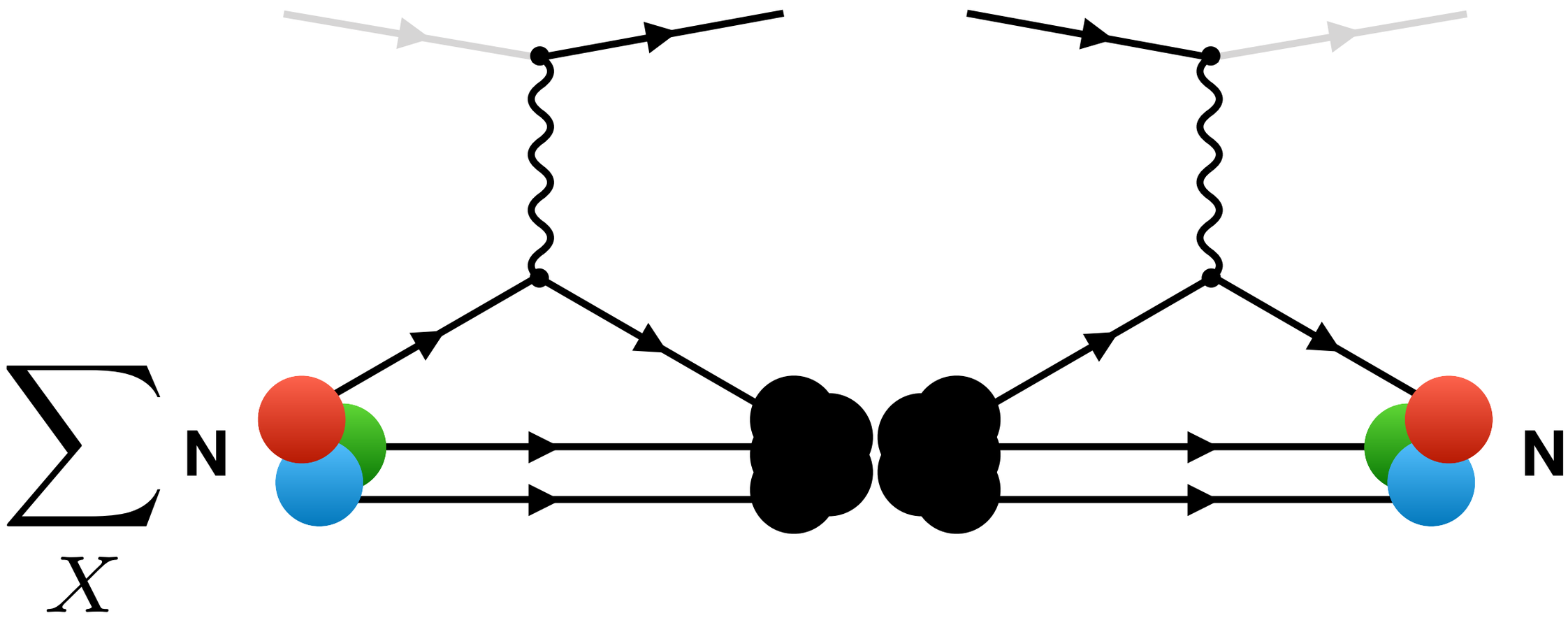


Sum over all possible hadronic final states X=N, Nπ, ...

Shallow Inelastic Scattering

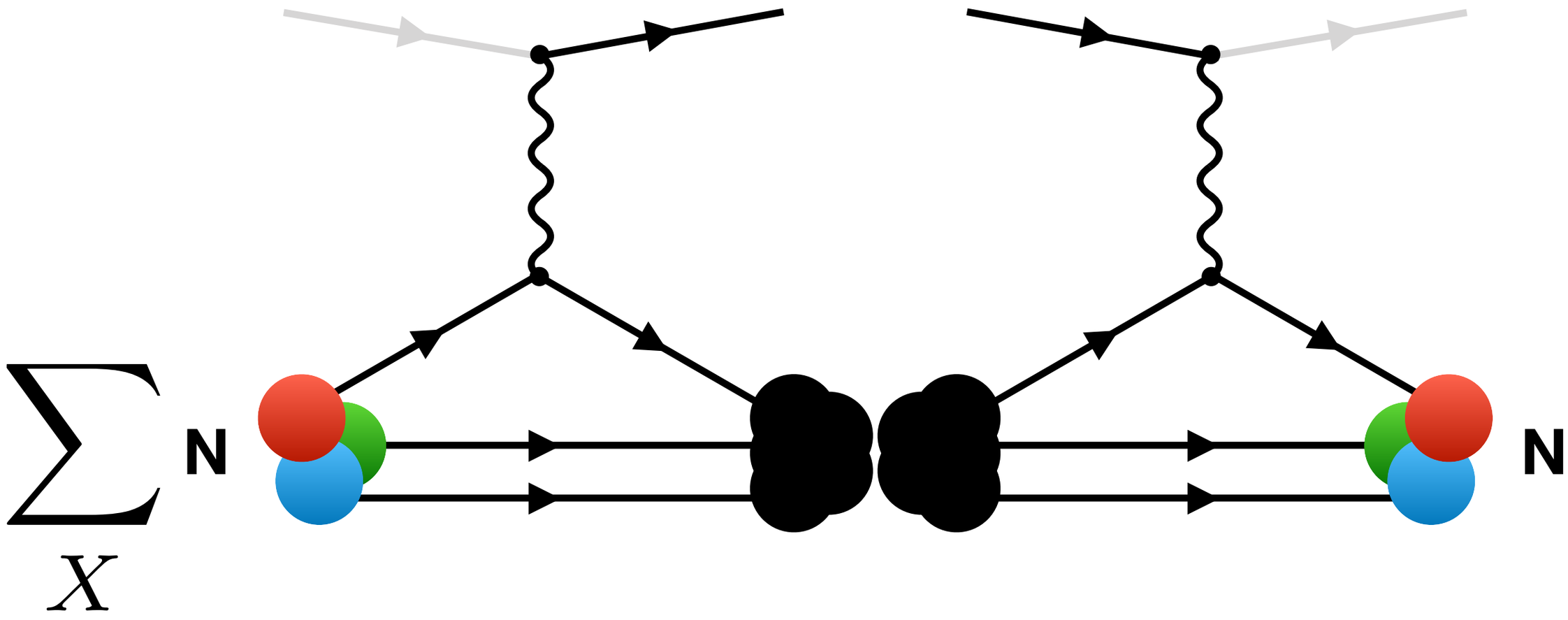
- The cross section is what's measured experimentally

$$\sigma \propto \mathcal{M}\mathcal{M}^\dagger$$



Shallow Inelastic Scattering

- In quantum mechanics: $\sum_X |X\rangle \langle X| = 1$

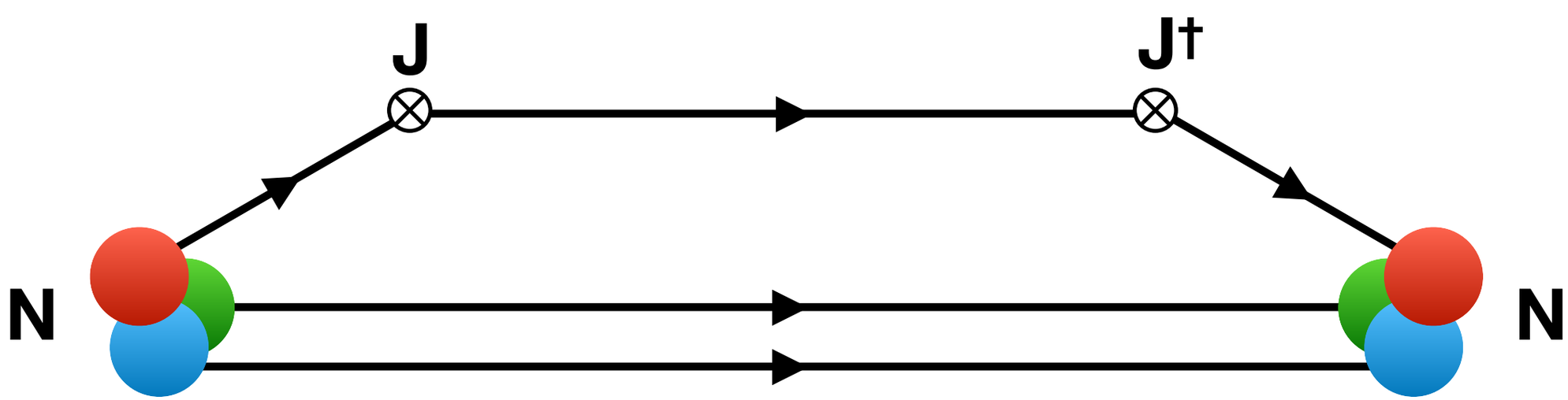


Shallow Inelastic Scattering

- Focus on QCD correlation function:

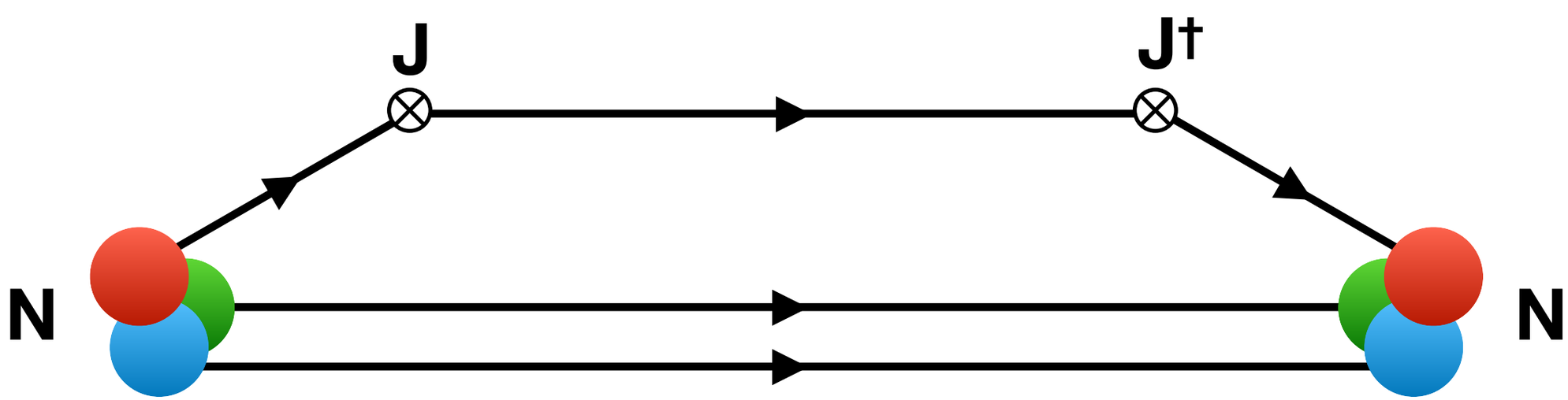
$$\langle N| J_\mu J_\nu^\dagger |N\rangle \propto W_{\mu\nu}$$

- $W_{\mu\nu}$ is the ***hadronic tensor***
- $W_{\mu\nu}$ related to structure functions, spectral densities



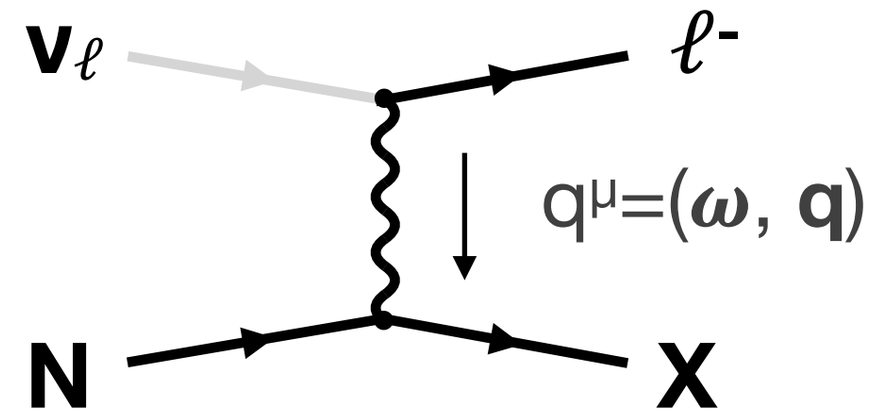
Shallow Inelastic Scattering

- Shallow inelastic scattering with many open channels ⟺ Non-perturbative QCD 4-point function
- Sum over all channels *automatically* included
- Let's try to compute it using lattice QCD



The physical hadronic tensor

- Physical cross sections



$$\sigma(E_\nu) = \int d\mathbf{q}^2 \int d\omega K(\omega, \mathbf{q}) W(\omega, \mathbf{q})$$

K = Kernel function

- Lepton tensor
- Propagator from W^+
- Phase space factors

W = Hadronic tensor

Need: $W(\omega, \mathbf{q})$

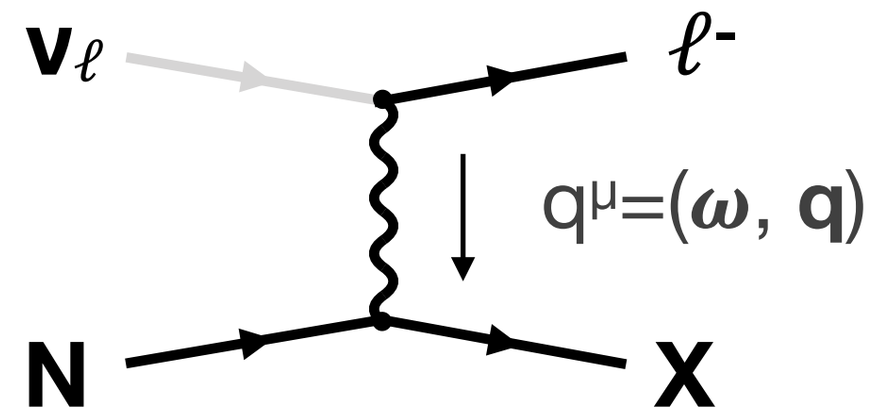
LQCD gives: $W(t, \mathbf{q})$

The physical hadronic tensor

- Must “Wick rotate” back to physical kinematics
- “Wick rotation” ⟺ Inverse Laplace transform

$$W(t, \mathbf{q}) = \int_0^\infty d\omega\, W(\omega, \mathbf{q}) e^{-\omega t}$$

LHS: Euclidean RHS: physical



- Numerically: Integral equation → Matrix equation

$$W(t_i) = T_{ij} W(\omega_j)$$

Strictly speaking, the problem is ill-posed: T_{ij} is not square ($i \ll j$)

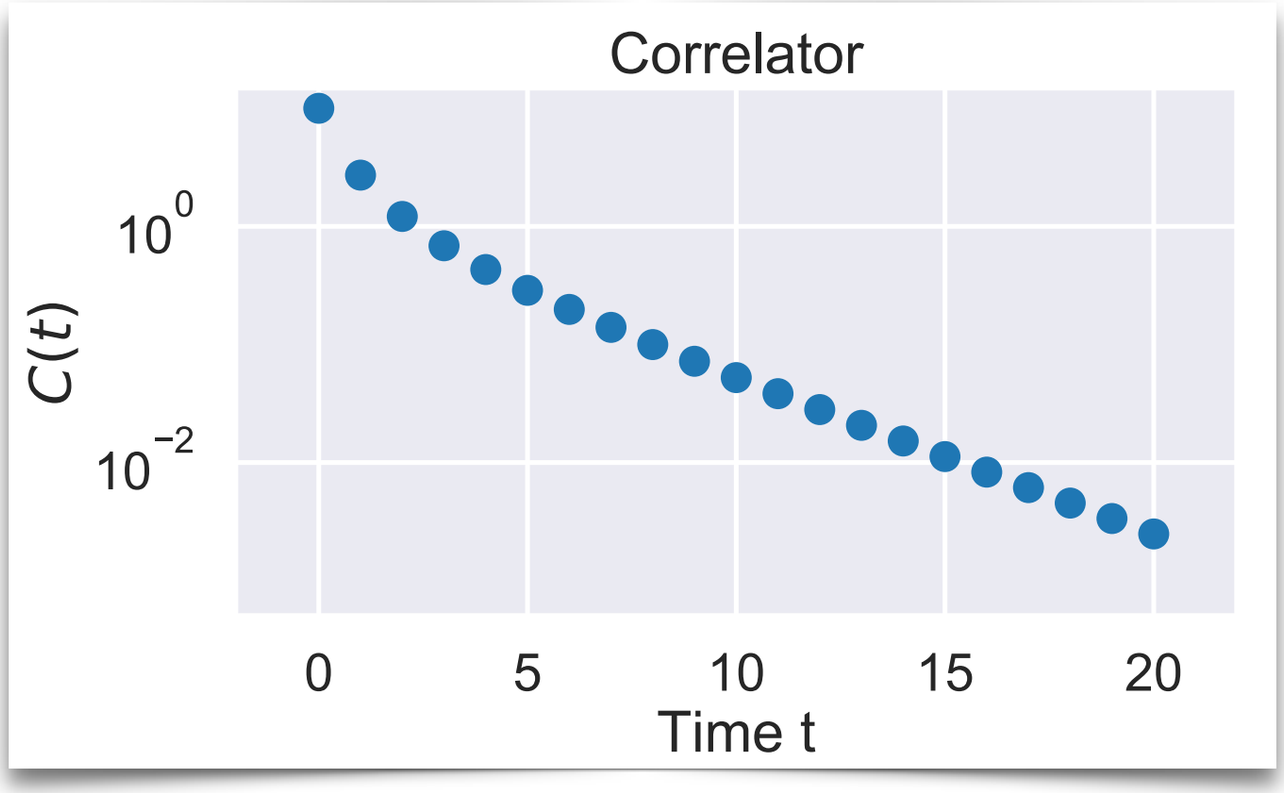
The physical hadronic tensor

- Practical proposals must somehow “regulate” the ill-posed numerical analysis problem with additional physics knowledge

- Before tackling this problem, let’s go back to thinking about quantum mechanics in a box.

Quantum Mechanics in a Box

$$C(t) = \sum_n |Z_n|^2 e^{-E_n t}$$

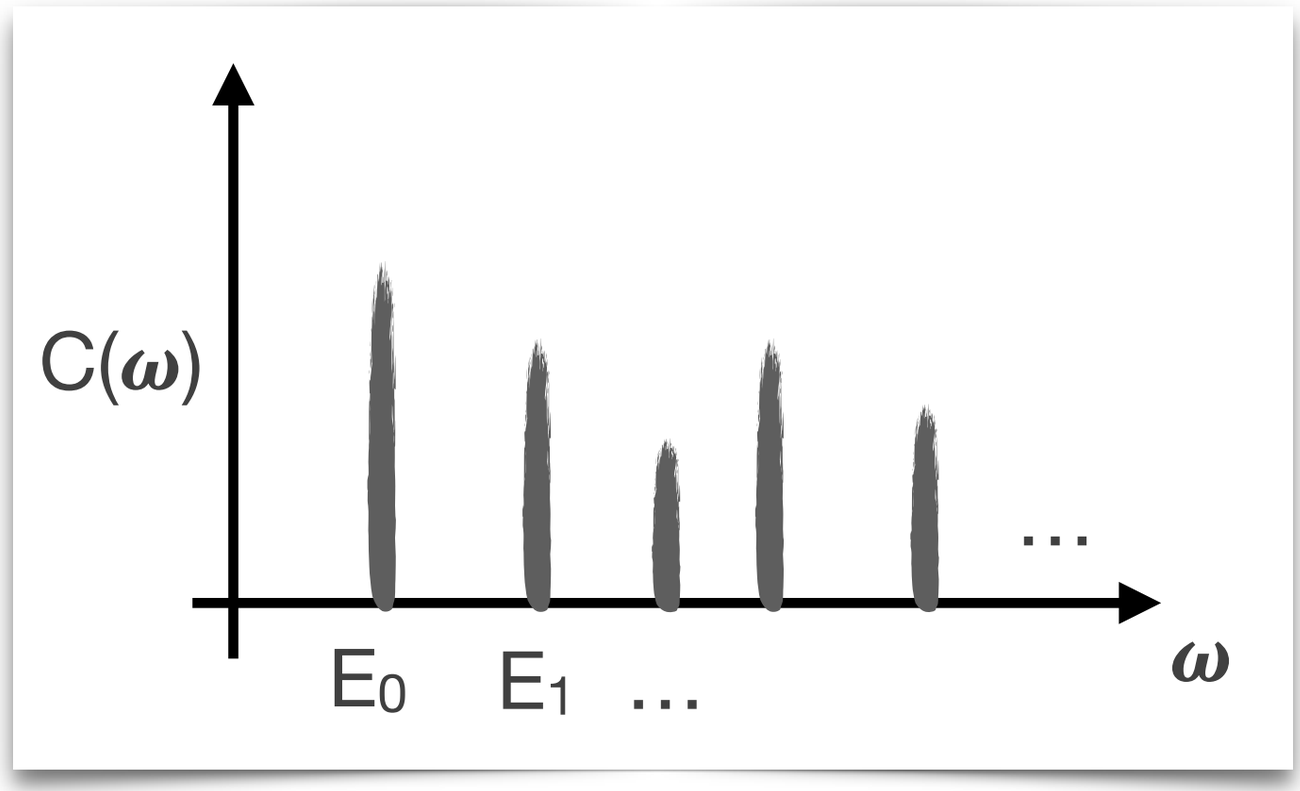


Quantum Mechanics in a Box

$$C(t) = \sum_n |Z_n|^2 e^{-E_n t}$$

Laplace transform

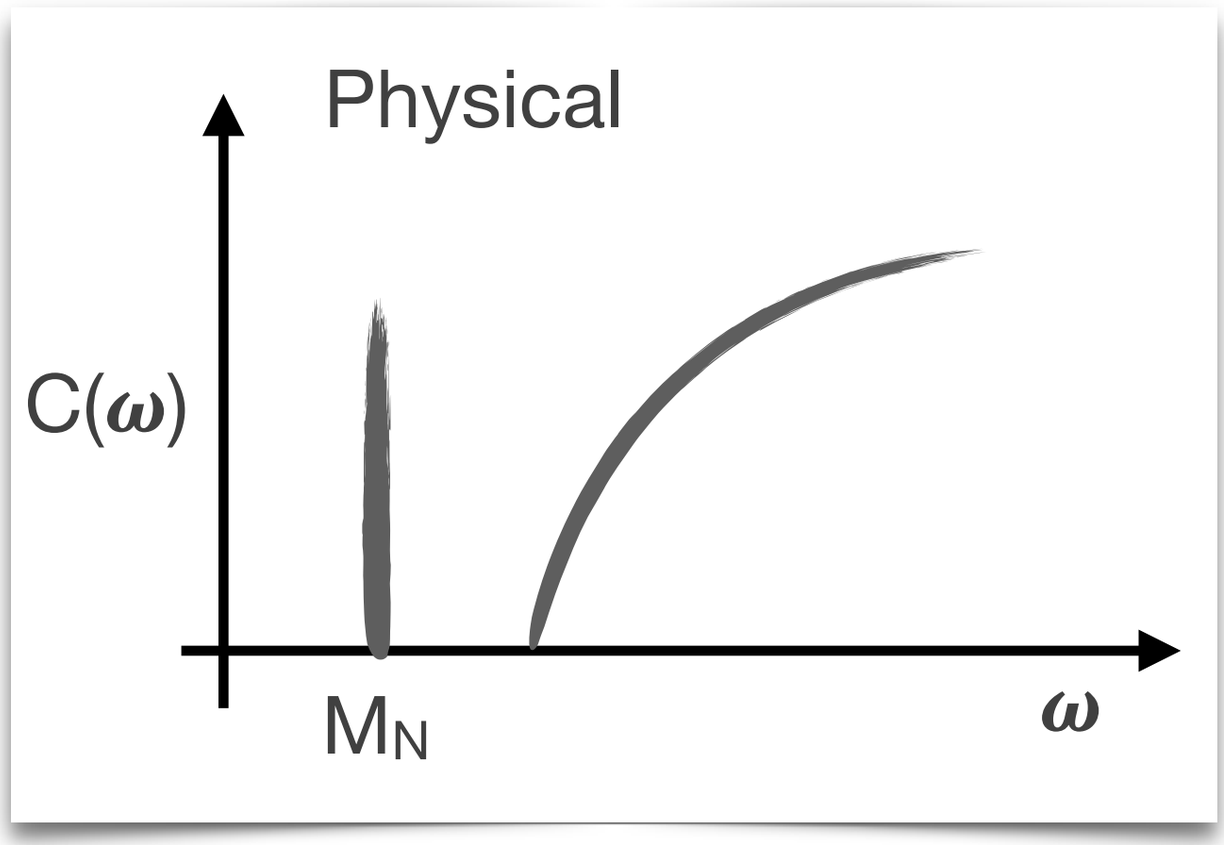
$$C(\omega) = \sum_n |Z_n|^2 \delta(\omega - E_n)$$

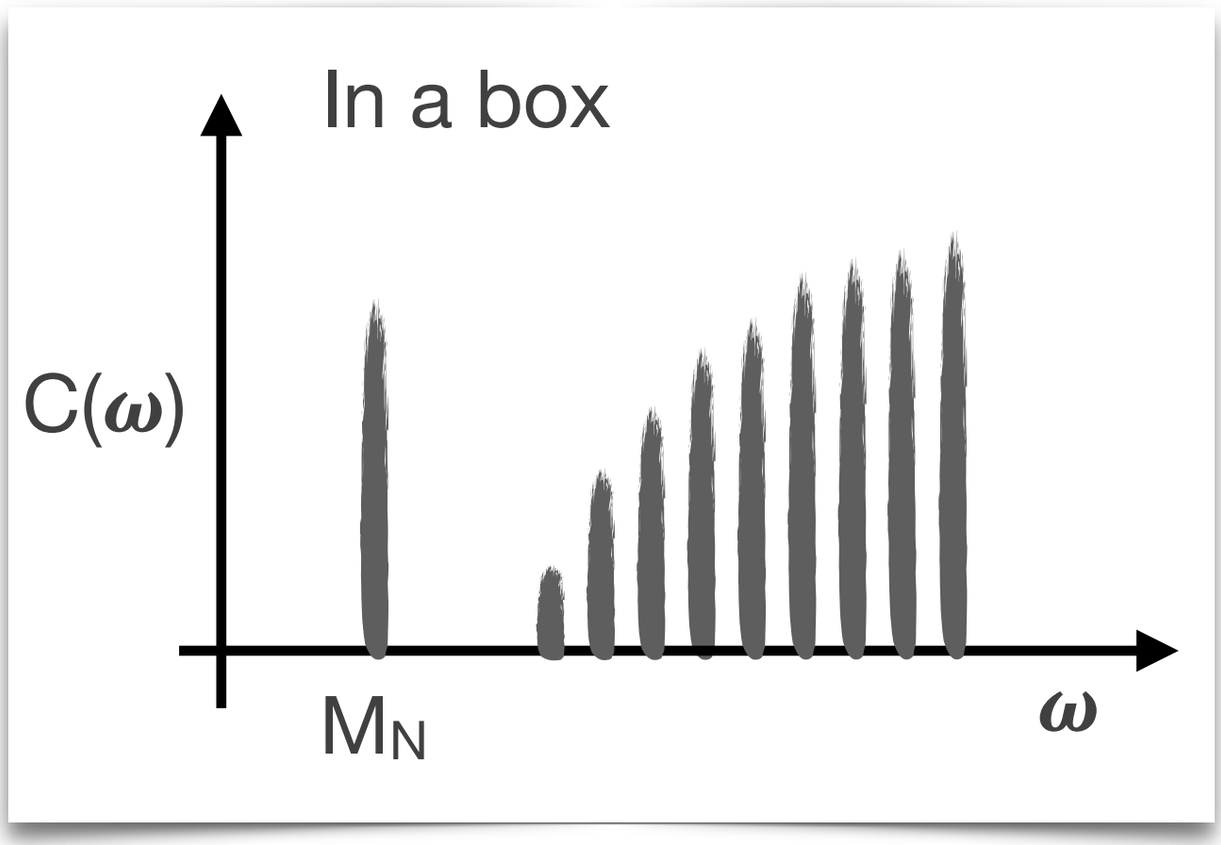


- “Spectral density” is Dirac comb, spike at each level
- This situation is completely generic
- Systems in a box have discrete energy levels

Quantum Mechanics in a Box

- What about hadronic tensor W($\boldsymbol{\omega}$, **q**)?
- Elastic channel: $\propto \delta(\omega - M_N)$
- Inelastic theshold: $\propto \Theta(\omega - M_N - M_\pi) \times (\text{phase space})$





Quantum Mechanics in a Box

- Somehow must connect these two pictures
- Try smearing
- (Actual methods will be different, but a classic idea)

PHYSICAL REVIEW D VOLUME 13, NUMBER 7 1 APRIL 1976

Smearing method in the quark model*

E. C. Poggio, H. R. Quinn,† and S. Weinberg
Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138
(Received 8 December 1975)

We propose that perturbation theory in a gauge field theory of quarks and gluons can be used to calculate physical mass-shell processes, provided that both the data and the theory are smeared over a suitable energy range. This procedure is explored in detail for the process of electron-positron annihilation into hadrons. We show that a smearing range of 3 GeV^2 in the squared center-of-mass energy should be adequate to allow the use of lowest-order perturbation theory. The smeared data are compared with theory for a variety of models. It appears to be difficult to fit the present data with theory, unless there is a new charged lepton or quark with mass in the region 2 to 3 GeV.

Approaches to the inverse problem

1. Backus-Gilbert reconstruction
   - Hansen, Meyer, and Robaina
   - [**arXiv:1704.08993**] PRD 96 (2017) 9, 094513
2. Orthogonal polynomials
   - Fukaya, Hashimoto, Kaneko, and Ohki
   - [**arXiv:2010.01253**]
3. Machine learning
   - Raghavan, Balaprakash, Lovato, Rocco, and Wild
   - [**arXiv:2010.12703**]

Approaches to the inverse problem

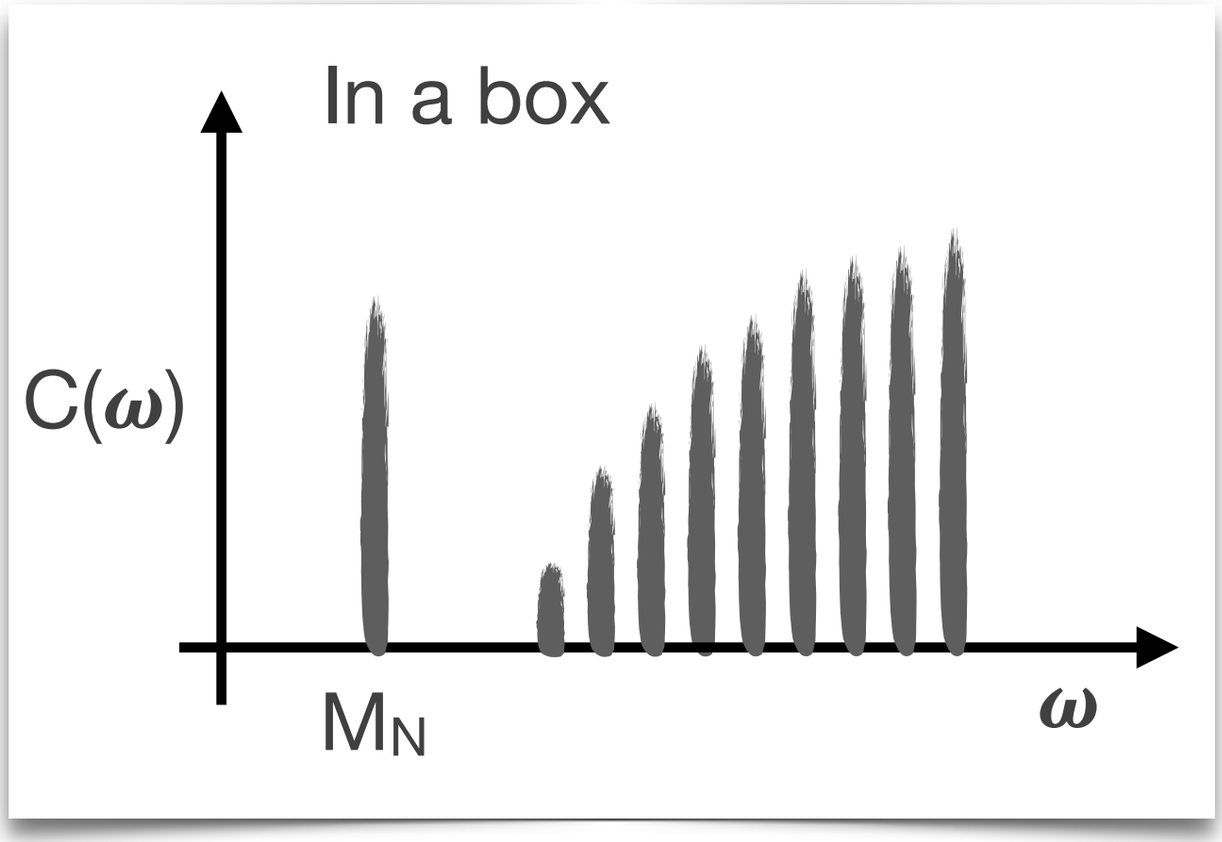
1. Backus-Gilbert reconstruction
   - Hansen, Meyer, and Robaina
   - [**arXiv:1704.08993**] PRD 96 (2017) 9, 094513
2. Orthogonal polynomials
   - Fukaya, Hashimoto, Kaneko, and Ohki
   - [**arXiv:2010.01253**]
3. Machine learning
   - Raghavan, Balaprakash, Lovato, Ro
   - [**arXiv:2010.12703**]

Today's talk

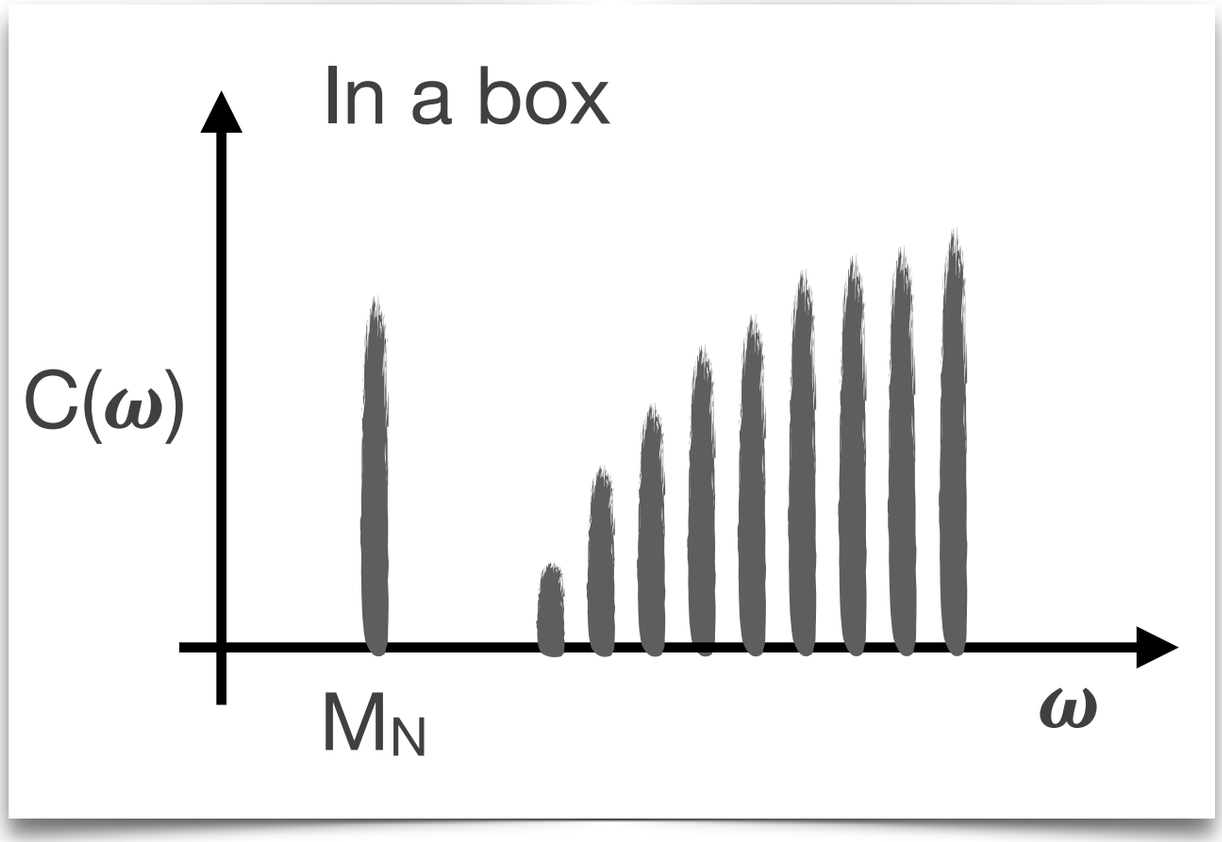
Very neat, but a discussion for another day

Backus-Gilbert Reconstruction

Backus-Gilbert reconstruction



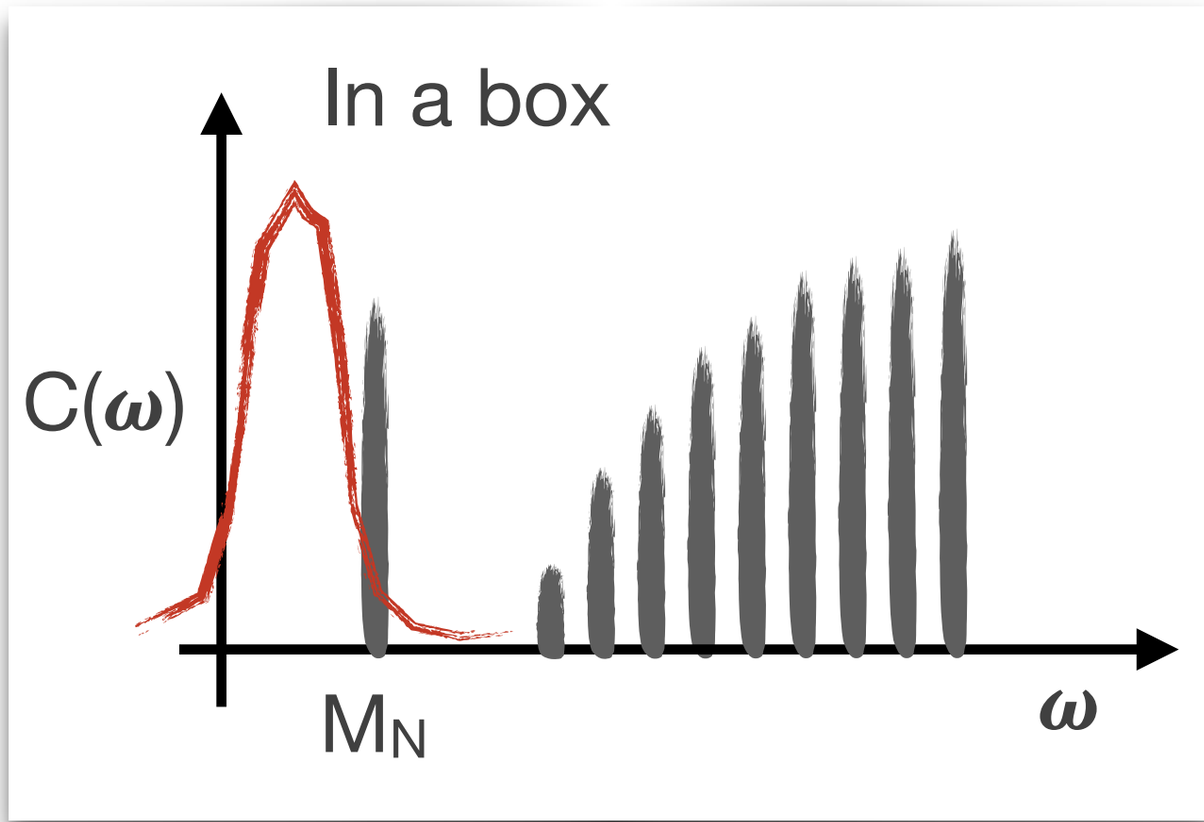
Backus-Gilbert reconstruction



$$= \delta_\Delta(\omega, \omega')$$

Smearing kernel = Regulated $\boldsymbol{\delta}$-function

Backus-Gilbert reconstruction

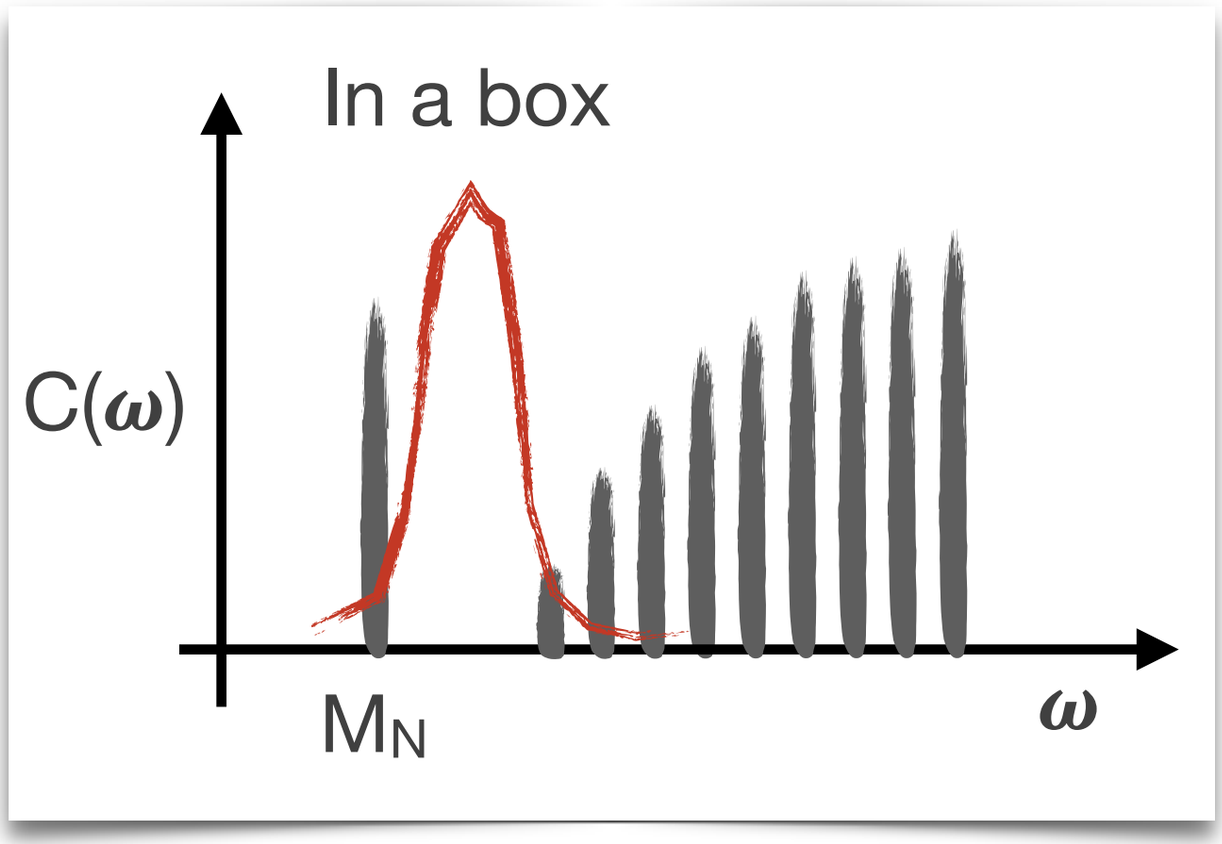


$$= \delta_\Delta(\omega, \omega')$$

$$C_\Delta(\omega) = \int d\omega' \, \delta_\Delta(\omega, \omega') C(\omega')$$

Smearing kernel = Regulated $\boldsymbol{\delta}$-function

Backus-Gilbert reconstruction

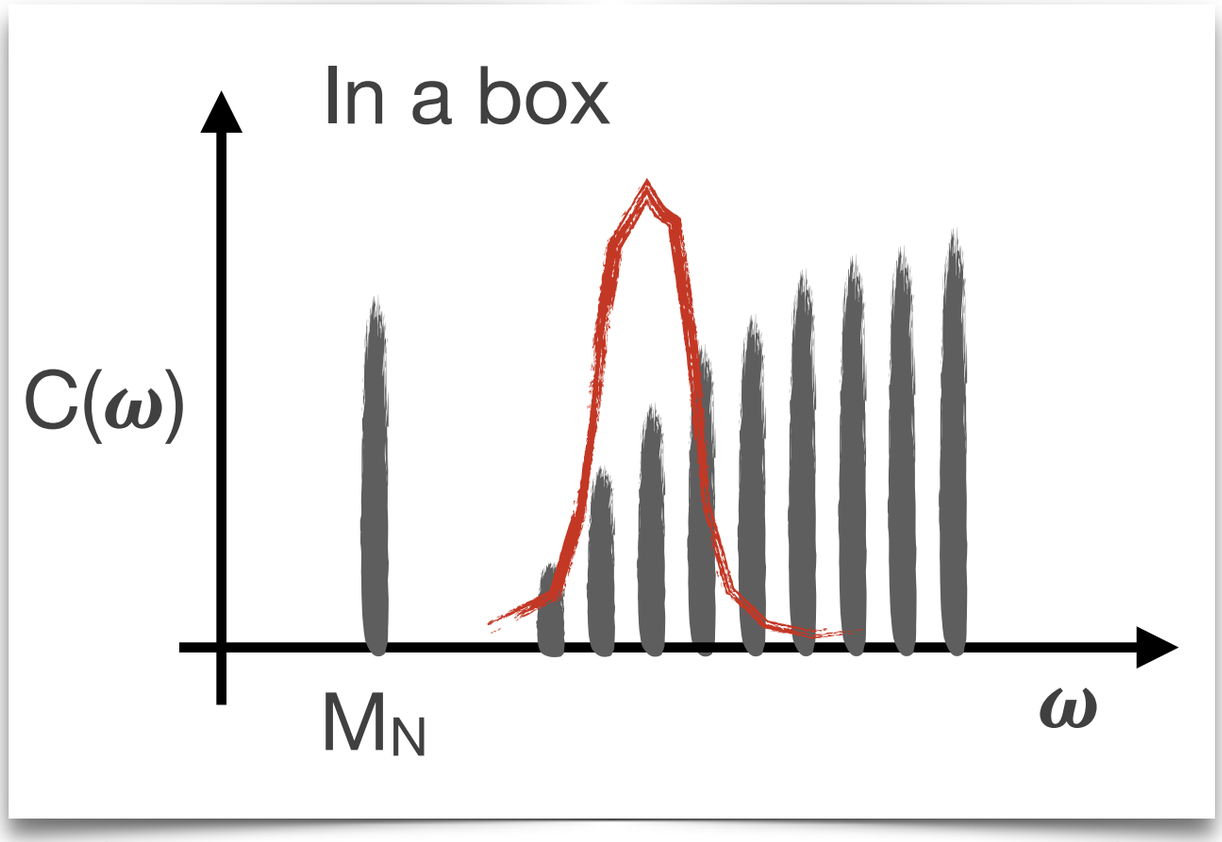


$$= \delta_\Delta(\omega, \omega')$$

$$C_\Delta(\omega) = \int d\omega' \, \delta_\Delta(\omega, \omega') C(\omega')$$

Smearing kernel = Regulated $\boldsymbol{\delta}$-function

Backus-Gilbert reconstruction

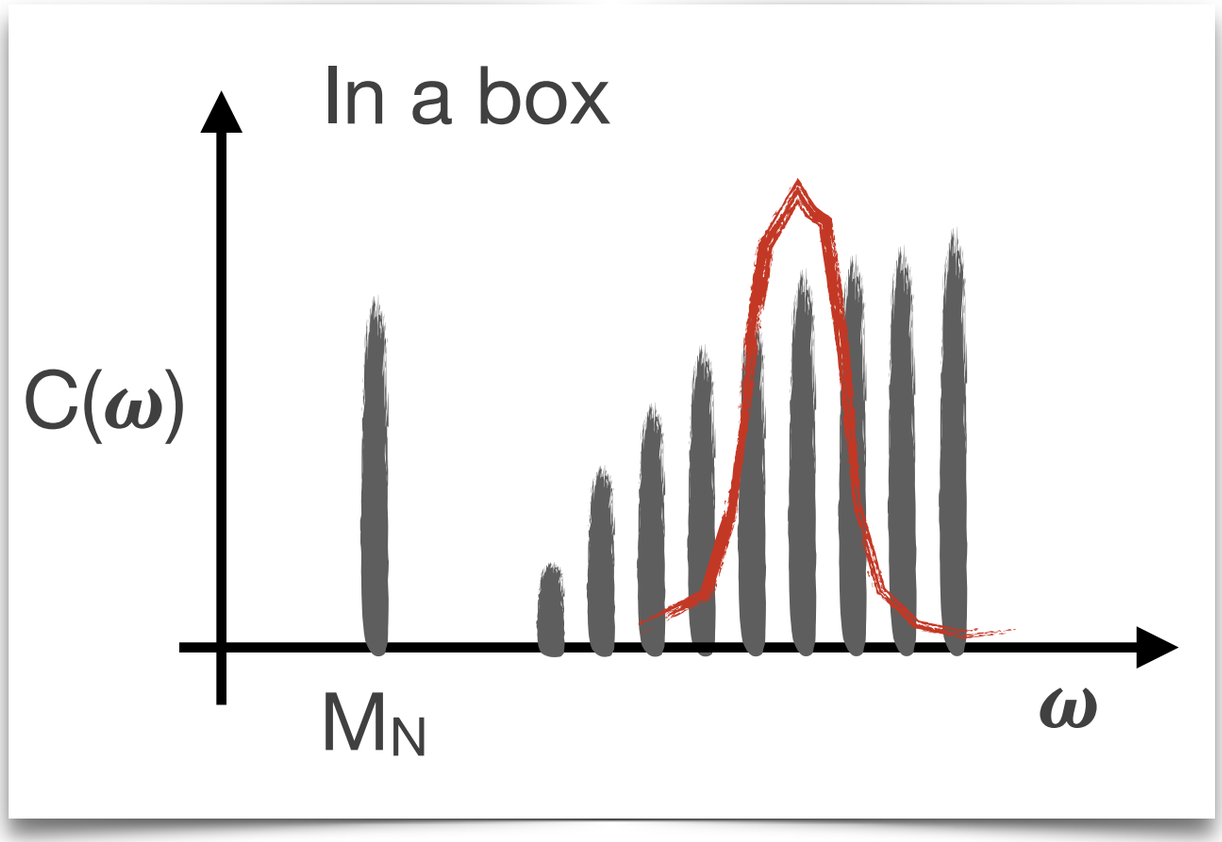


$$= \delta_\Delta(\omega, \omega')$$

$$C_\Delta(\omega) = \int d\omega' \, \delta_\Delta(\omega, \omega') C(\omega')$$

Smearing kernel = Regulated $\boldsymbol{\delta}$-function

Backus-Gilbert reconstruction

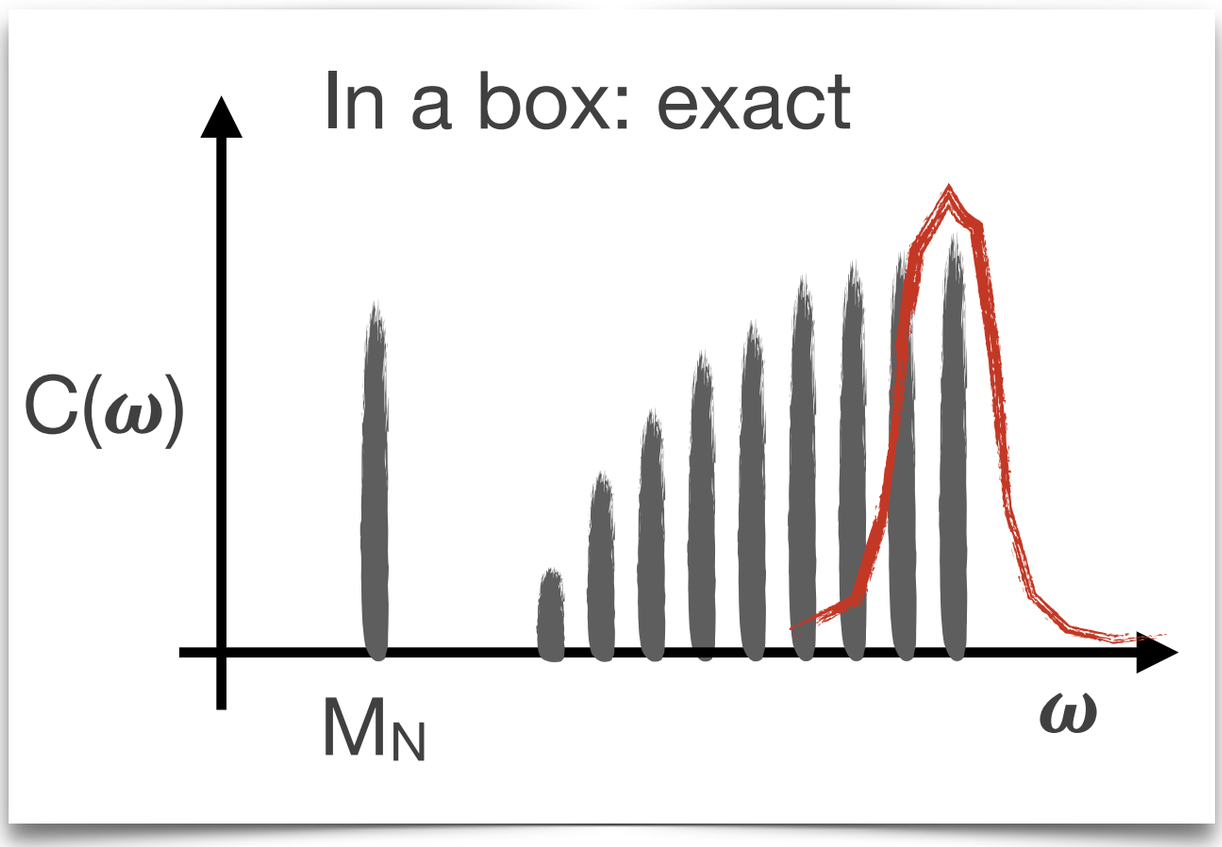


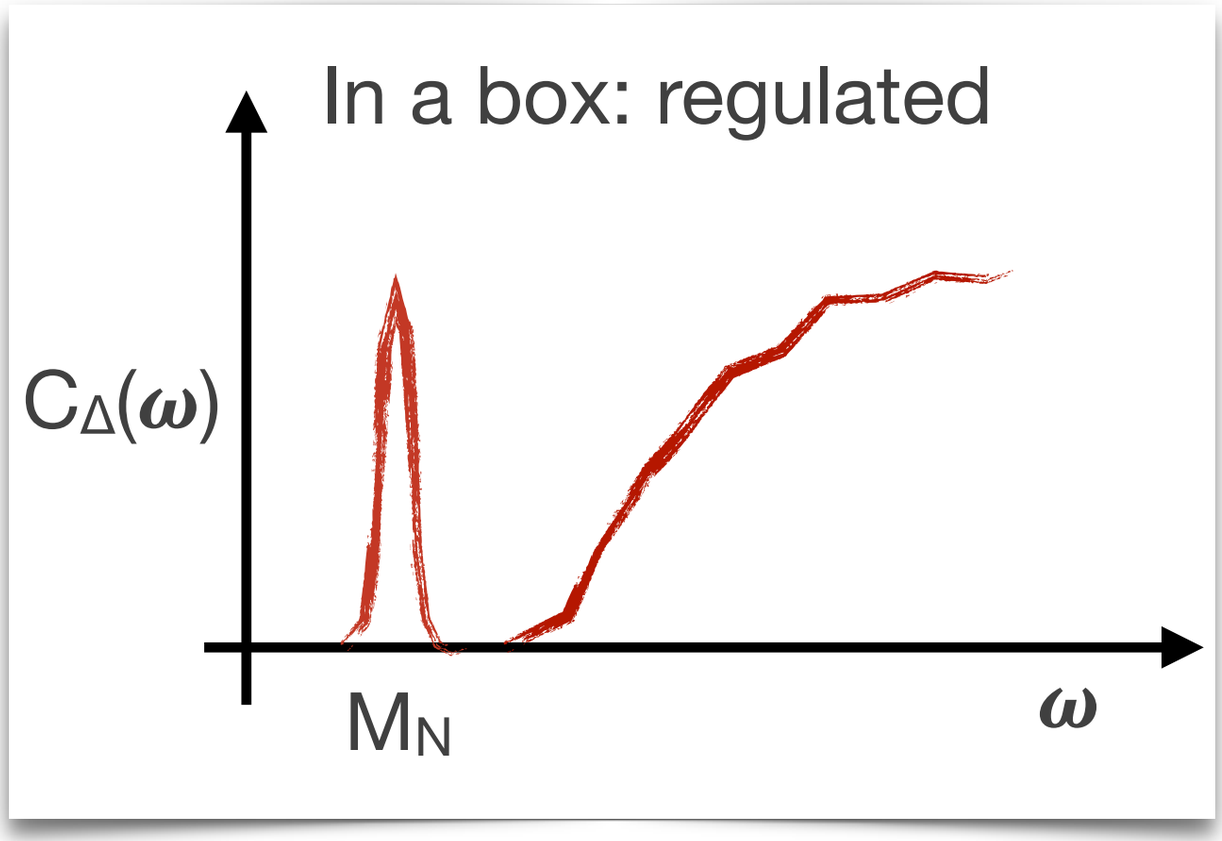
$$= \delta_\Delta(\omega, \omega')$$

$$C_\Delta(\omega) = \int d\omega' \, \delta_\Delta(\omega, \omega') C(\omega')$$

Smearing kernel = Regulated $\boldsymbol{\delta}$-function

Backus-Gilbert reconstruction



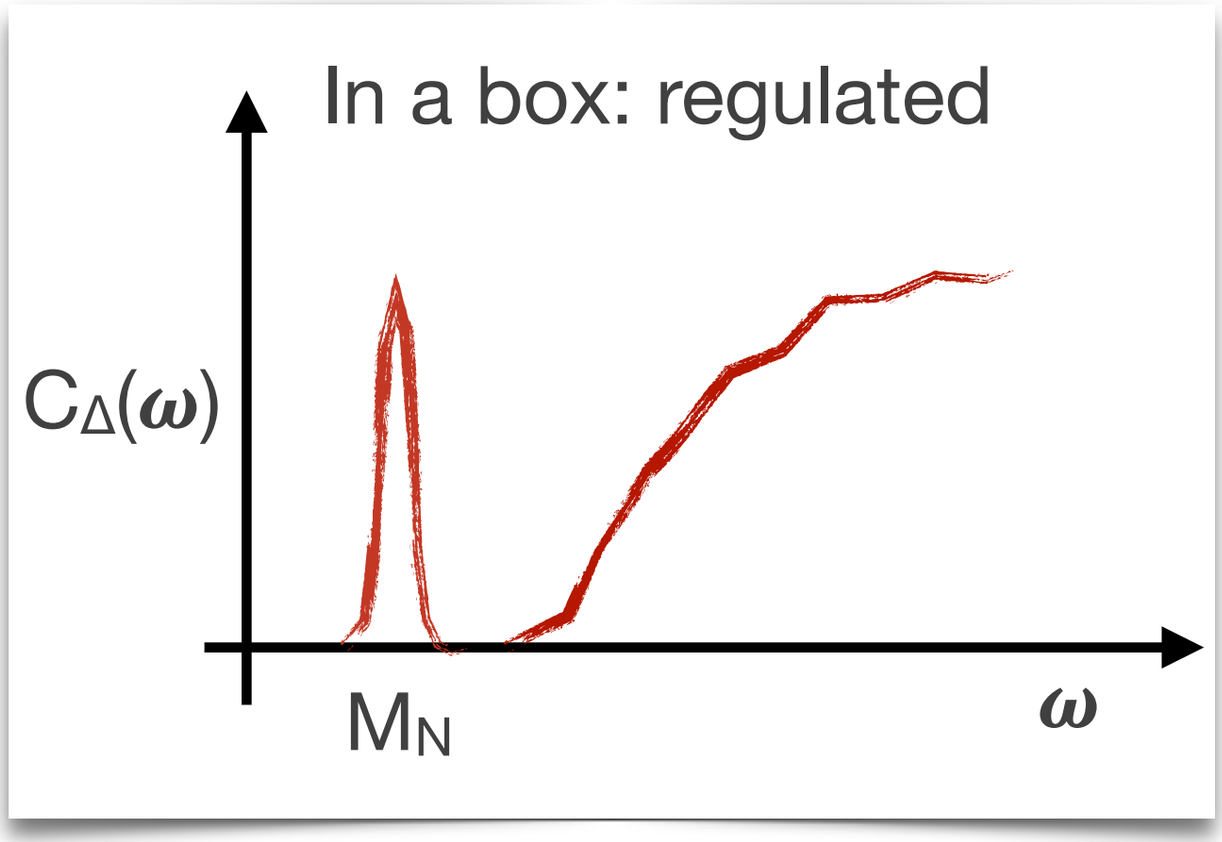


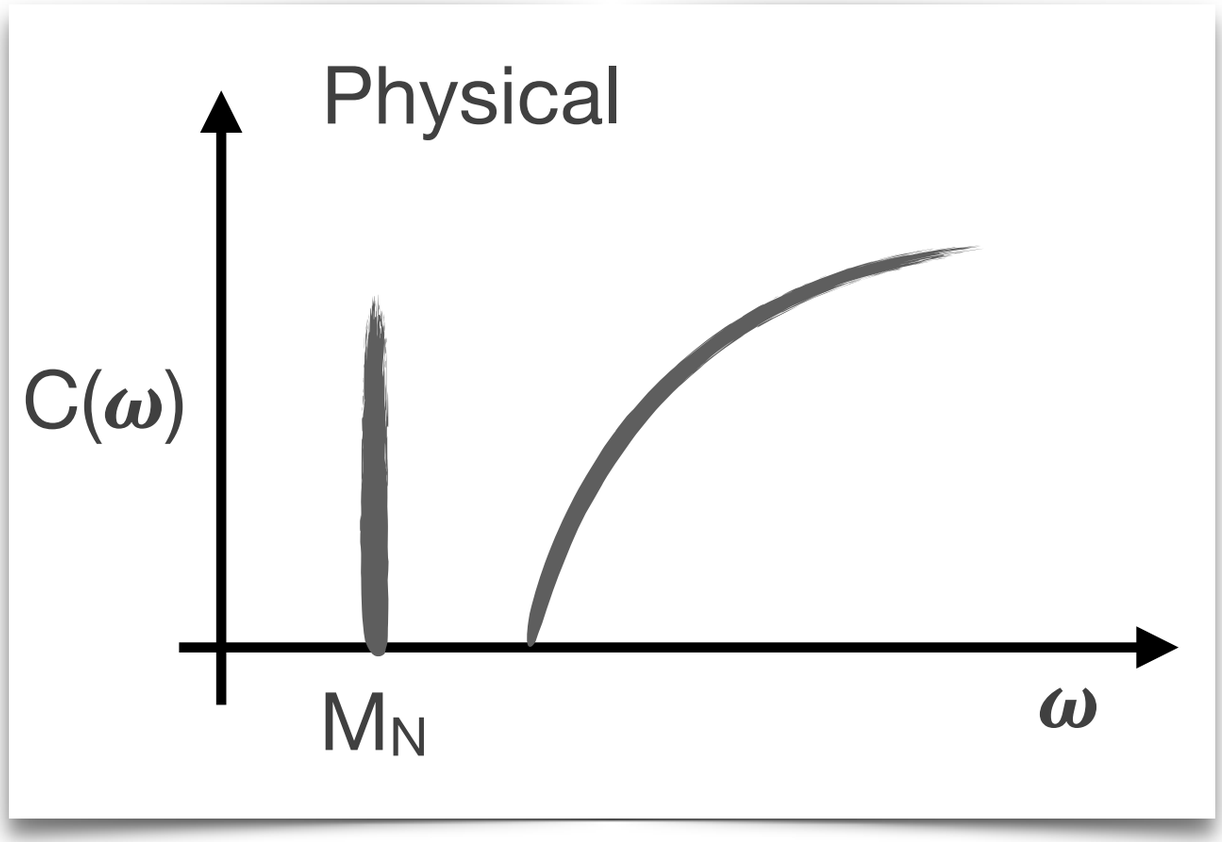
$$= \delta_\Delta(\omega, \omega')$$

$$C_\Delta(\omega) = \int d\omega' \, \delta_\Delta(\omega, \omega') C(\omega')$$

Smearing kernel = Regulated $\boldsymbol{\delta}$-function

Backus-Gilbert reconstruction





- Take limit to reach physical result

$$\lim_{\Delta\to 0}\ \lim_{\mathrm{box}\to\infty} C_\Delta(\omega) \longrightarrow C(\omega)$$

Backus-Gilbert reconstruction

- Ill-posed nature of unregulated problem $\Longleftrightarrow$

  Results are very sensitive to small changes in data
- Phrase inversion problem as convex optimization
- "Find smearing kernel $\boldsymbol{\delta}_\Delta$ which minimizes width Δ"
- Then work with smeared function $C_\Delta(\boldsymbol{\omega})$
- Upshots:

  ☑ Smearing regulates and stabilizes the inversion

  ☑ Smearing connects finite-volume to continuum

Orthogonal Polynomials

Orthogonal Polynomials

- Experiments measure cross sections, not $W_{\mu\nu}$

$$\sigma(E_\nu) = \int d\mathbf{q}^2 \int d\omega K(\omega, \mathbf{q}) W(\omega, \mathbf{q})$$

K = Kernel function

- Lepton tensor
- Propagator from W^+
- Phase space factors

W = Hadronic tensor

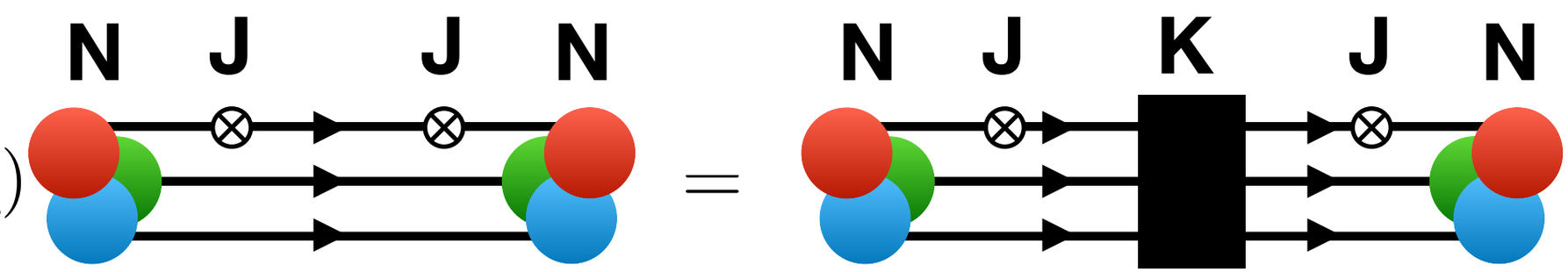
Note: K is known analytically. Can we leverage this?

Orthogonal Polynomials

- Experiments measure cross sections, not $W_{\mu\nu}$
- It turns out: (standard QM tricks)

$$\int d\omega K(\omega, \mathbf{q}) W(\omega, \mathbf{q}) \; = \langle N | \, J(-\mathbf{q}) K(\hat{H}, \mathbf{q}) J(-\mathbf{q}) \, | N \rangle$$

$\int d\omega K(\omega, \mathbf{q})$

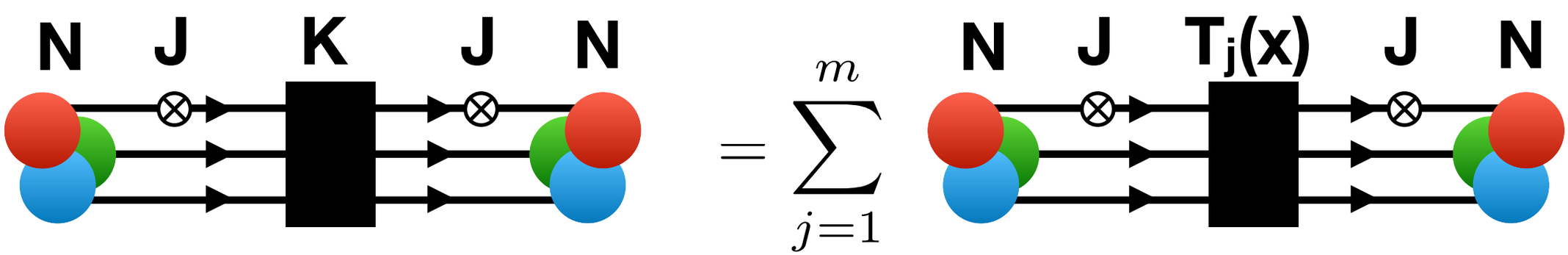


- This seems perverse. 4-point → 5-point function

Orthogonal Polynomials

- ***But,*** the kernel function K($\boldsymbol{\omega}$) is known analytically
- Let's expand in orthogonal polynomials $T_n(x)$

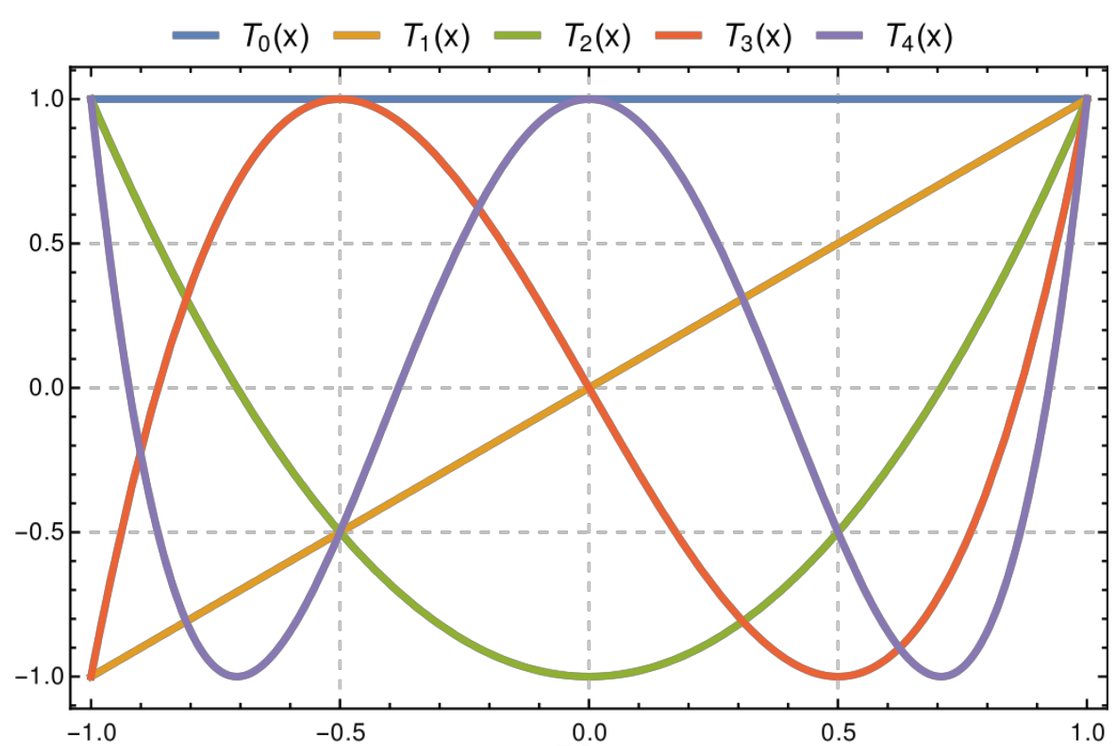
$$K(x) = c_0 + \sum_{j=1}^{m} c_j T_j(x)$$



- Still a 5-point function… are we winning?

Orthogonal Polynomials

- We started with $K(\omega)$. May as well use $K(e^{-\omega})=K(x)$
- Energies are positive, so $e^{-\omega} = x$ in [0,1]
- Q: What is a good approximation for K(x)?
- A: Try expanding in Chebyshev polynomials.

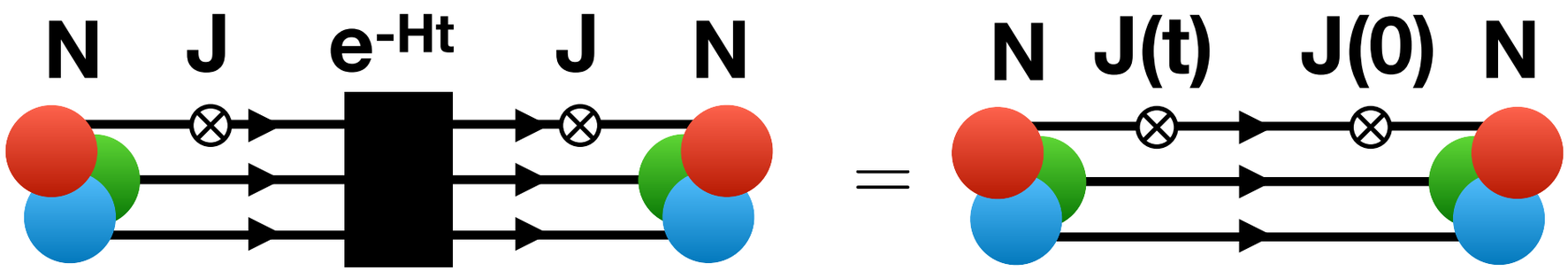


Orthogonal Polynomials

- We started with $K(\omega)$. May as well use $K(e^{-H})=K(x)$
- Energies are positive, so $e^{-H} = x$ in [0,1]
- Q: What is a good approximation for f(x)?
- A: Try expanding in Chebyshev polynomials.
  - n-th order polynomials in x use 1, x, … x^n
  - $x= e^{-H}$, so actually need 1, e^{-H}, … e^{-nH}
- But e^{-Ht} is just Euclidean time evolution!

Orthogonal Polynomials

- In other words,



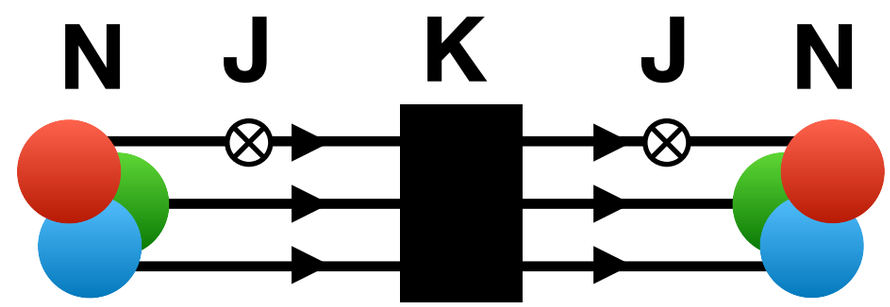
e^{-HT} gives Euclidean time evolution between abstract states $J|N\rangle$

Use currents with Euclidean time separation t

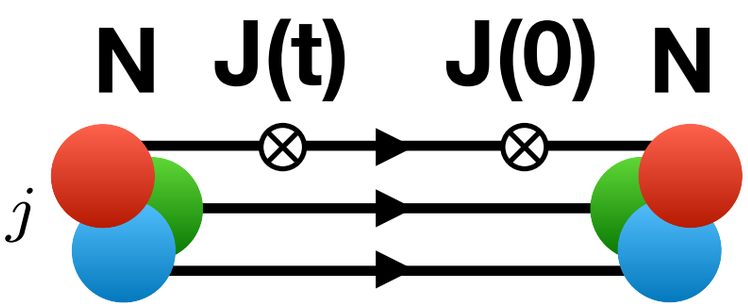
Orthogonal Polynomials

- What have we won for ourselves?
- Wanted cross section $\sigma(E_\nu) = \int d\mathbf{q}^2 \int d\omega K(\omega, \mathbf{q}) W(\omega, \mathbf{q})$
- We found:

$$\int d\omega K(\omega, \mathbf{q}) W(\omega, \mathbf{q}) =$$



$$= \sum_{t=1}^{j} (\#)_j$$



LHS: Needs hadron tensor for *physical* kinematics

RHS: Can compute using lattice QCD. j different times gives j^{th}-order approx.

Orthogonal Polynomials

- What have we won for ourselves?
- Wanted cross section $\sigma(E_\nu) = \int d\mathbf{q}^2 \int d\omega K(\omega, \mathbf{q}) W(\omega, \mathbf{q})$
- We related the integrated hadronic tensor to

  Euclidean matrix elements → Can use lattice QCD!
- Upshots:

☑ The "4pt→5pt→4pt" tricks handles the inversion

☑ K($\boldsymbol{\omega}$,**q**) acts as a smearing kernel for finite volume

Looking ahead

Frontier calculations

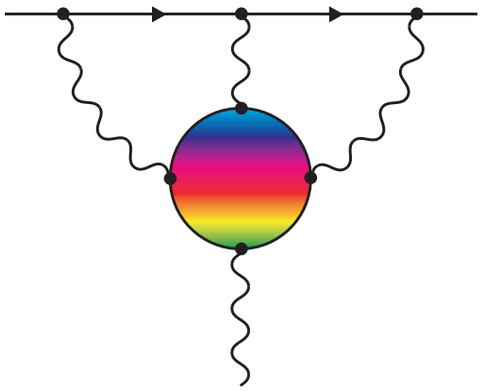
The physics of Euclidean correlation functions:

- 2-point functions: masses, decay constants ✓
- 3-point functions: form factors ✓

- 4-point functions:
  - Neutrino physics: shallow inelastic scattering, $0\nu\beta\beta$-decay
  - Flavor physics: Inclusive B-meson decays
  - Kaon physics: K_L-K_S mixing, ε_K, rare kaon decays
  - Hadron structure: $H_{\mu\nu}$

Questions for the future

- How to compute the 4-point functions?
  - They are numerically challenging
  - See HLbL for (g-2) for state of the art



- Which inversion techniques work well in practice?
  - Current studies have mostly considered toy data
  - Will they perform well on real Monte Carlo data?

- Baryons are generically difficult
  - Baryons have challenging signal-to-noise properties
  - Good solutions needed for many different systems

Summary

- Grounding νA scattering in QCD is important
- Finding BSM physics requires careful theoretical understanding of the Standard Model itself
- Lattice QCD can provide benchmarks at all the energy scales relevant to the DUNE program
- Non-perturbative shallow inelastic scattering is theoretically challenging
- New ideas (algorithmic and theoretical) in lattice QCD make the shallow inelastic region very exciting
- Experimental demands are driving these efforts, and I expect big progress over the next 5-10 years

Backup slides

Numerical challenges

- Each fermion line is a propagator S
- Propagators = Inverse of Dirac matrix

3x colors a,b at source and sink

4x spins α,β at source and sink

V total sites x, y

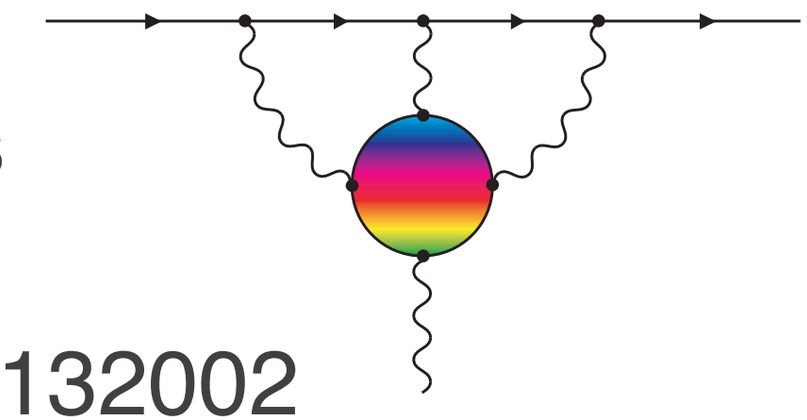
$$S^{ab}_{\alpha\beta}(x|y)$$

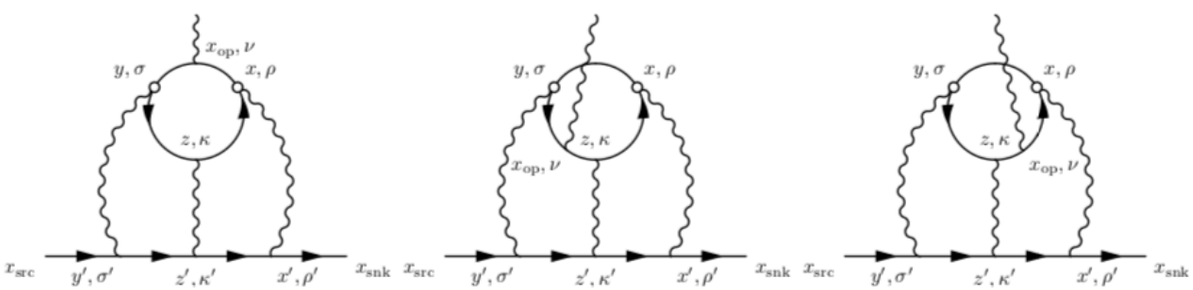
Full matrix has $O(V^2)$ total entries

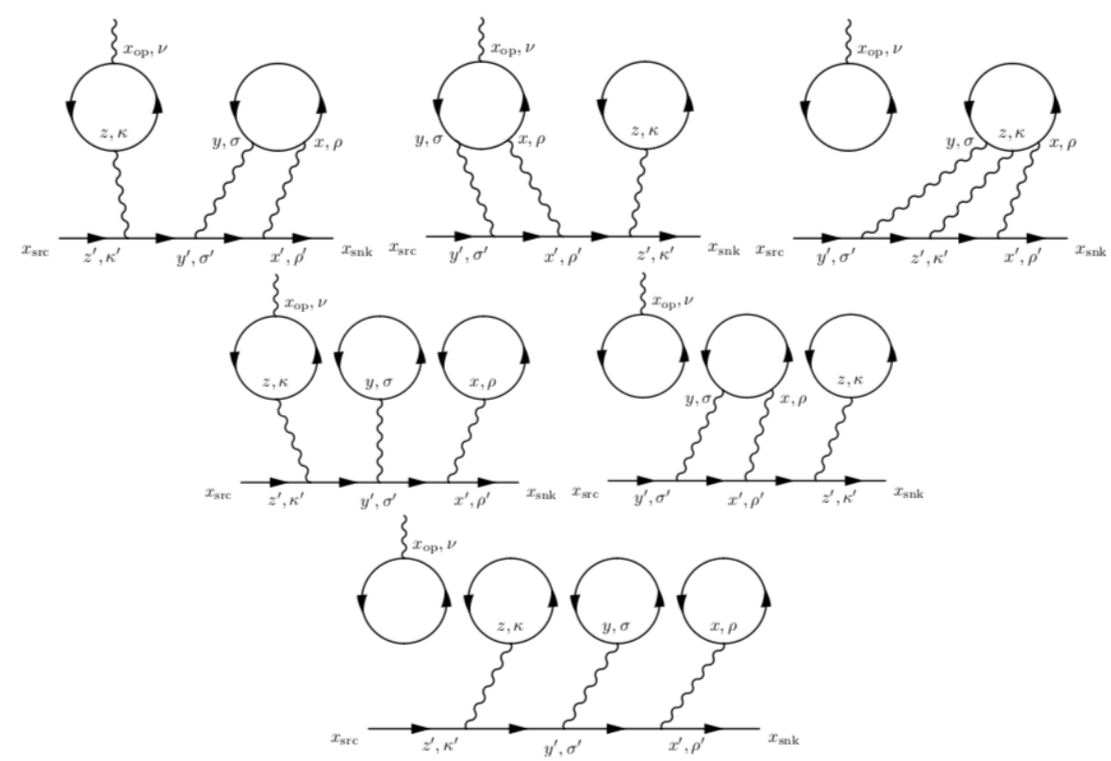
- As usual: Avoid solving Ax=b numerically with A^{-1}
- Use tricks (= physics knowledge) to be more clever

Numerical challenges

- Hadronic light-by-light scattering
  - Proof-of-concept for 4-pt functions
  - Not just a toy problem
  - T. Blum et al, PRL 124 (2020) 13, 132002
  - **[arXiV:1911.08123]**







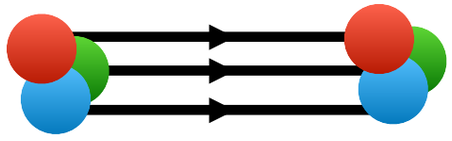
Baryons are hard

- Baryons (e.g., nucleons) are extended objects
  - Overlap with simple point-like objects is often poor
  - Challenge: find a good basis of interpolating operators to achieve flat effective mass curves at early times
  - Related: FNAL Theory Seminar on 9/10/2020 by Amy Nicholson, “Advances in N-N scattering”

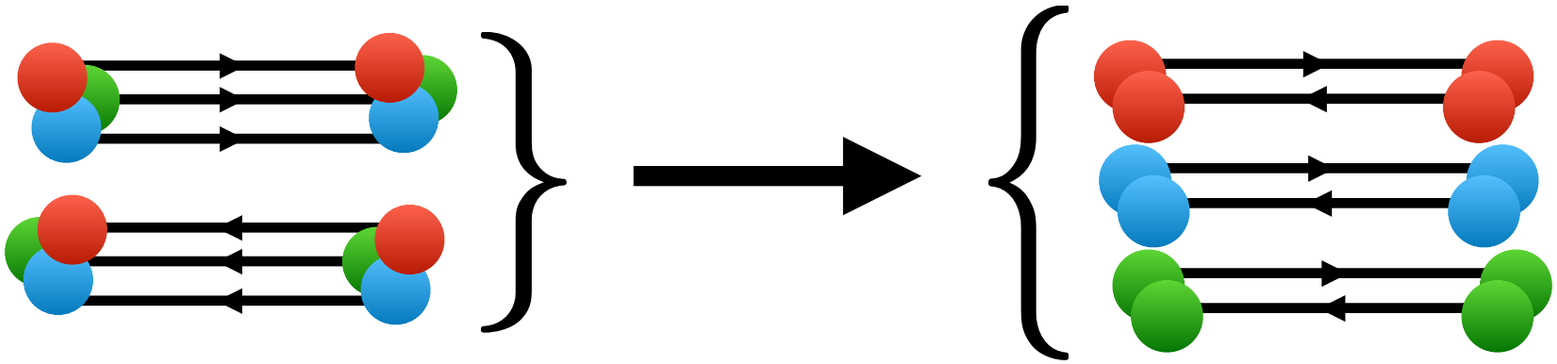
Baryons are hard

- Parisi-Lepage: Variance dominated by lowest-energy state with matching quantum numbers

$$\langle C_N(t)\rangle \sim e^{-m_N t}$$



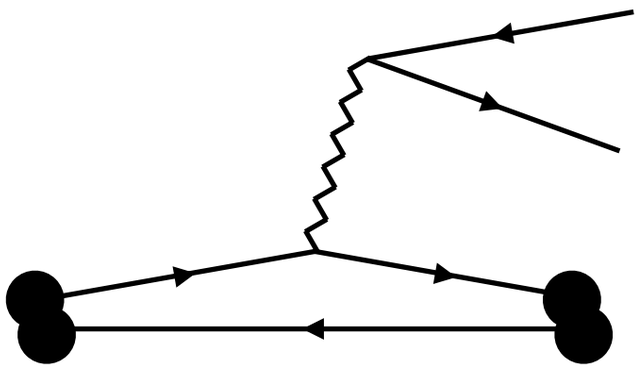
$$\mathrm{Var}(C_N) = \langle |C_N(t)|^2\rangle \sim e^{-3m_\pi t}$$



$$\frac{\text{Noise}}{\text{Signal}} = \frac{\sqrt{\mathrm{Var}(C_N)}}{C_N} \sim e^{(m_N - 3/2 m_\pi)t}$$

Exclusive Semi-leptonic Decays

Via numerical lattice QCD



(form factors) ∝ (matrix elements)

$$f_J(p) \propto \langle \text{final}| \, J(p) \, |\text{initial}\rangle$$

- Methodology is well established
- Systematic effects are well understood
- Calculations are underway using physical quark masses: u, d, s, c, and b.
- Coming soon:

» B-meson decay form factors at the 1% level

» D-meson decay form factors at sub-percent level