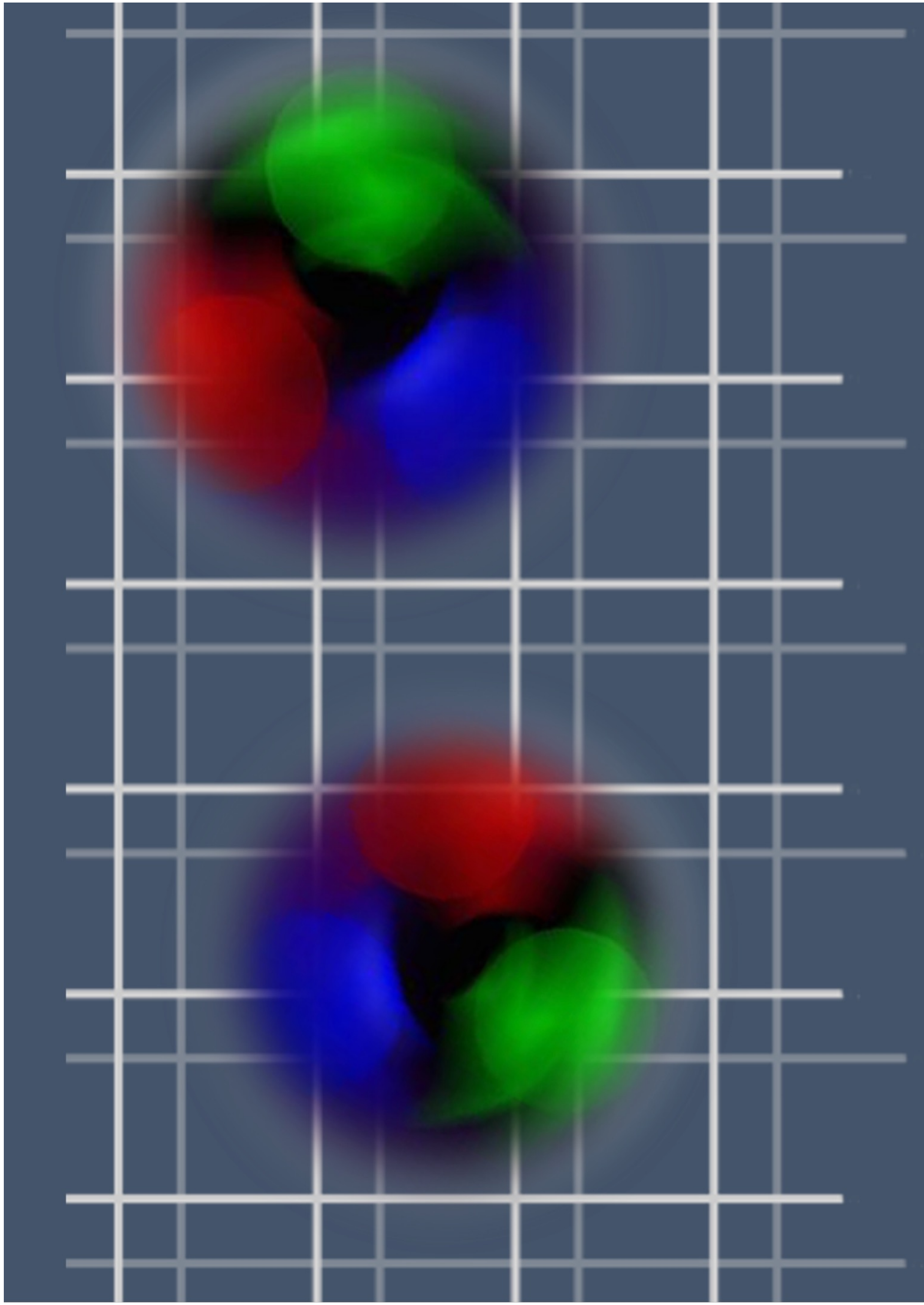

Lattice QCD

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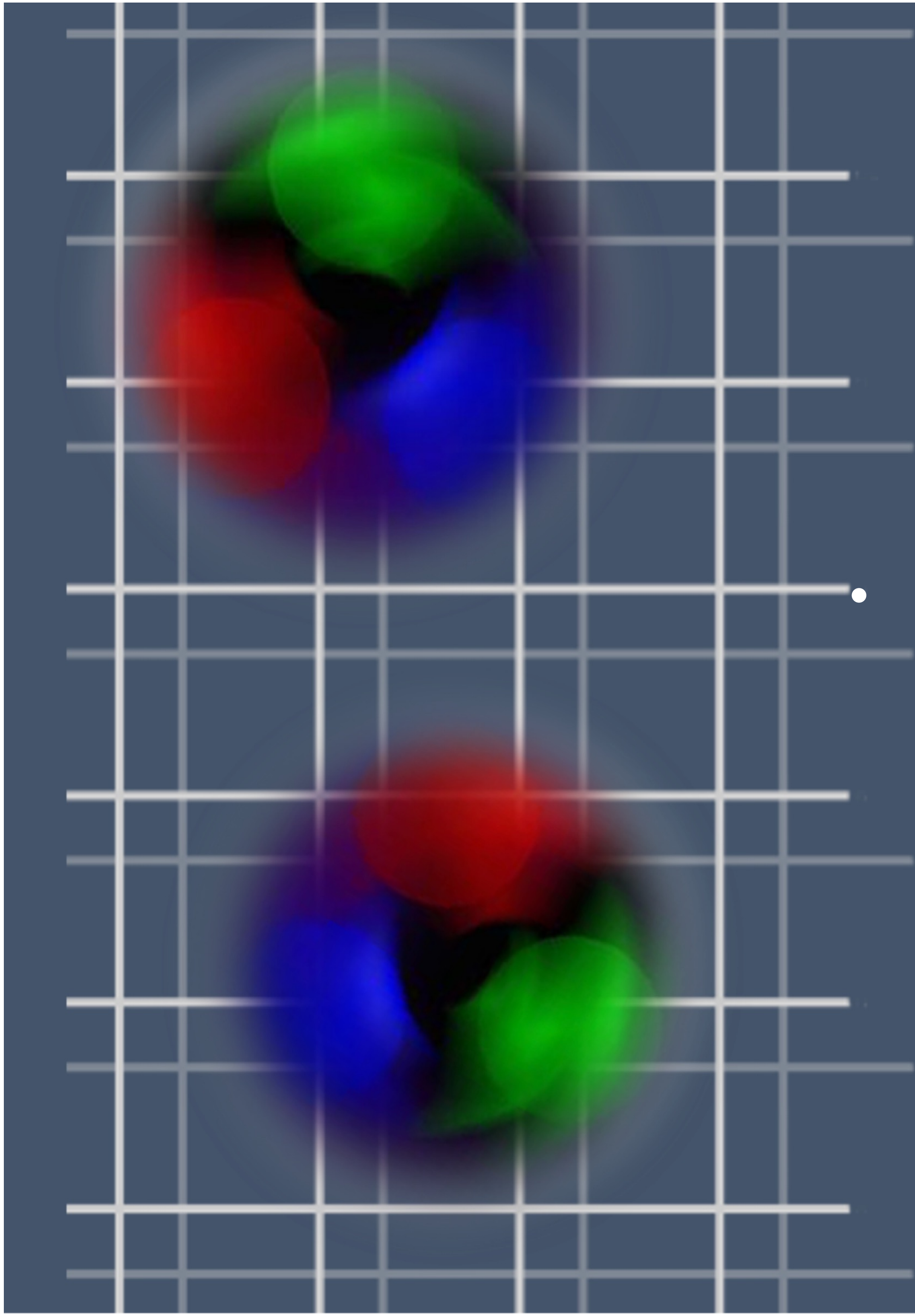
Benasque Science Center
September 04, 2024



CONTENTS

- Introduction
- Path-integral formalism
- Correlation functions
- Energy spectrum from LQCD
- Some applications

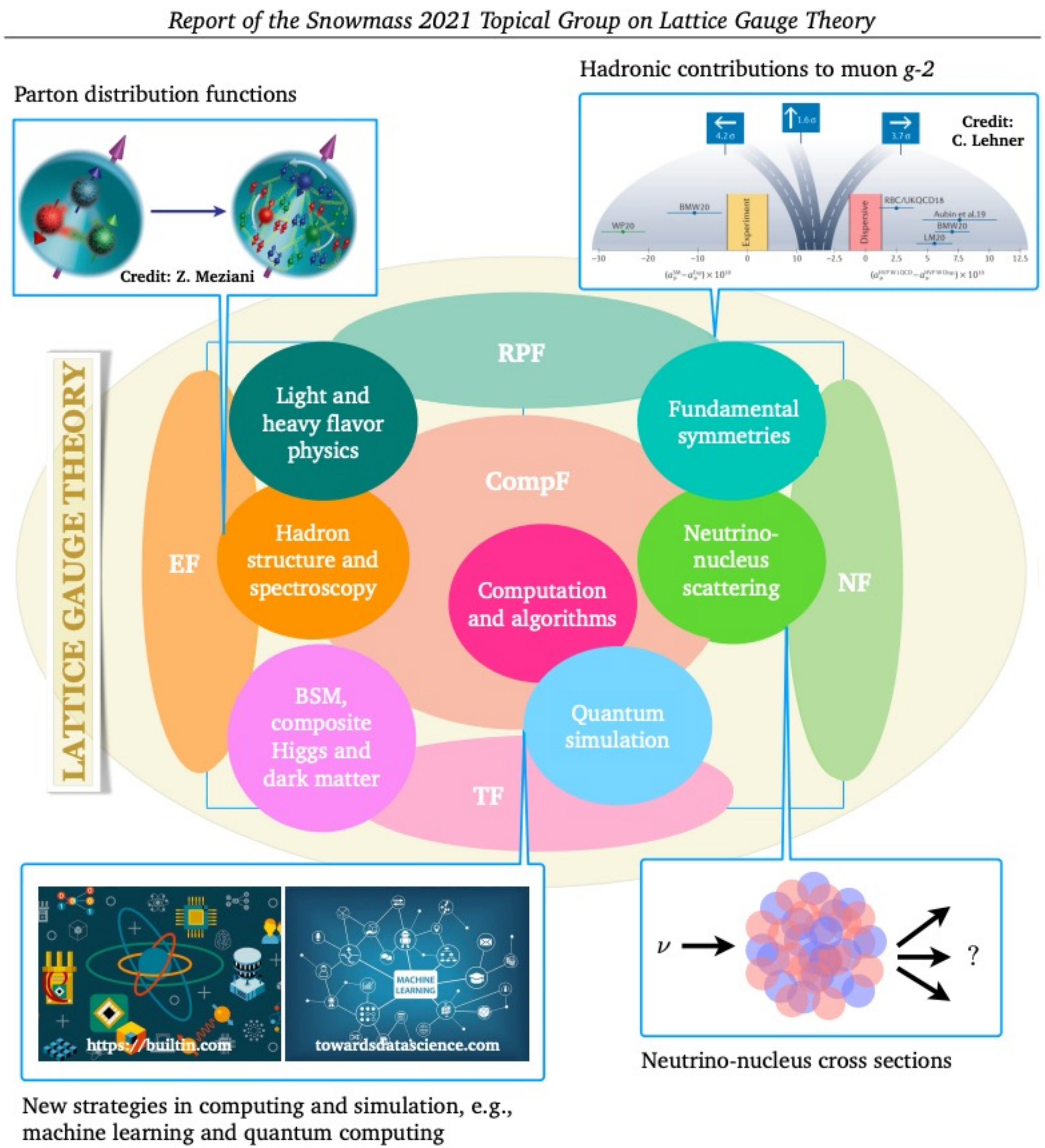
Tutorial:

Hadron masses

from LQCD calculations

Assumpta Parreño

Sandra Tomás



The lattice-gauge-theory program touches on many areas of research in HEP as classified within the topical Frontiers of Snowmass2021

TF: Theory Frontier
NF: Neutrino Frontier
RPF: Rare Processes and Precision Measurement Frontier
EF: Energy Frontier
CompF: Computational Frontier

Areas with high impact and/or high levels of innovation along with select examples are highlighted in the figure.

Powerful theoretical and computational approach to simulating strongly interacting quantum field theories

Applications permeate almost all disciplines of modern-day research in High-Energy Physics.

- to enable precision quark- and lepton-flavor physics (lattice high-energy physics effort aims to reduce QCD uncertainties to at-or-below measurement errors to maximize discovery potential of high-precision experiments)
- calculation of matrix elements to uncover signals of new physics in nucleons and nuclei (dark matter searches in cosmology...)
- to elucidate hadron structure and spectrum
- to serve as a numerical laboratory to reach beyond the Standard Model
- or to invent and improve state-of-the-art computational paradigms

Improvement in theoretical frameworks and algorithmic suits

QCD Lagrangian

$$\mathcal{L}_{QCD} = \bar{q}_{ij}\left(i\gamma^{u}\partial_{u} - m_{j}\right)q_{ij} + g(\bar{q}_{ij}\gamma^{u}\lambda_{a}q_{ij})F_{u}^{a} - \frac{1}{4}F_{uv}^{a}F_{a}^{uv}$$

with $i = r, g, b \quad j = u, d, c, s, t, b \quad q:\text{quark spinor}$

Interesting consequences come from the non-Abelian character of the SU(3) group:

1. Quarks are confined. We will never be able to "see" a quark as we see a proton or an electron. This explains why we have no direct experimental evidence for free quarks. **All hadrons (mesons and baryons) are color singlets.**

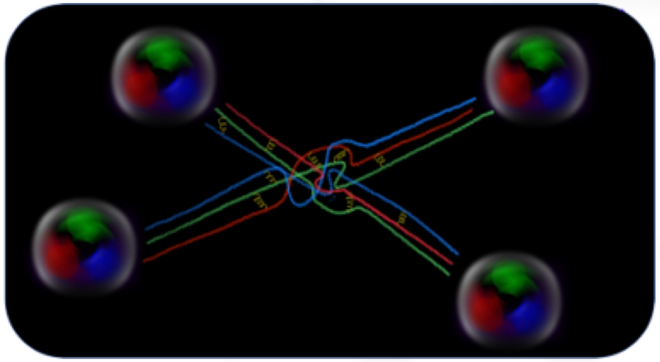
2. Asymptotic freedom. The coupling constant of QCD changes very rapidly with energy ("running coupling constant"). Consequently, the quarks appear free in lepton scattering experiments, where a high-energy virtual photon knocks a quark out of the hadron, but are strongly bound inside hadrons (low-energy).

3. Calculations in the nonperturbative regime of QCD are difficult.

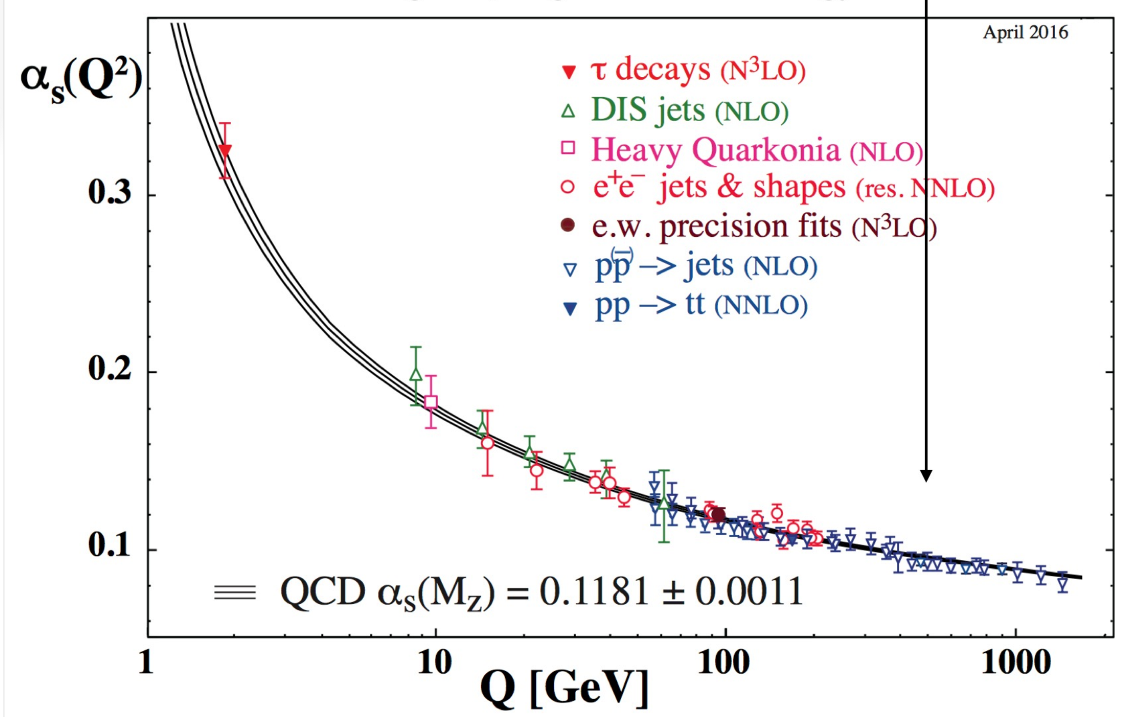
→ Look for approximate/simplified ways to perform the calculation (chiral perturbation theory, large-scale numerical calculations, etc.)

Nuclear physics, the non-perturbative regime of QCD

Perturbation theory applicable



strong coupling constant *vs* energy

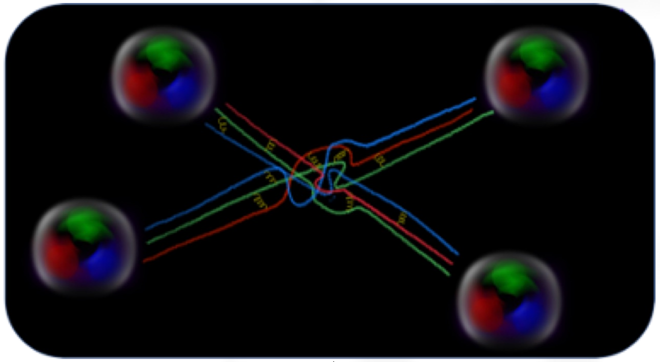


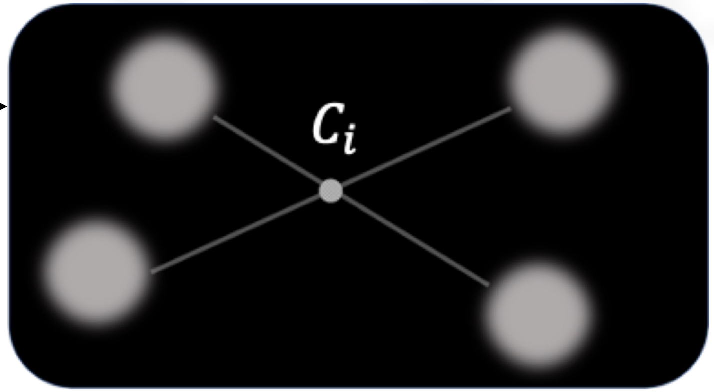
$$\mathcal{L}_{QCD} = \bar{q}_{ij}\left(i\gamma^u \partial_u - m_j\right)q_{ij} + g(\bar{q}_{ij}\gamma^u \lambda_a q_{ij})F_u^a - \frac{1}{4}F_{uv}^{a}F_{a}^{uv}$$

$$i = r,g,b \quad j = u,d,c,s,t,b$$

S. Bethke, G.Dissertori, G.P. Salam
EPJ Web of Conferences 120 07005 (2016)

Absence of analytical solutions of QCD in the nonperturbative regime





$$\mathcal{L}_{QCD} = \bar{q}_{ij}\left(i\gamma^{u}\partial_{u} - m_{j}\right)q_{ij} + g(\bar{q}_{ij}\gamma^{u}\lambda_{a}q_{ij})F_{u}^{a} - \frac{1}{4}F^{\,a}_{uv}F^{\,uv}_{a}$$

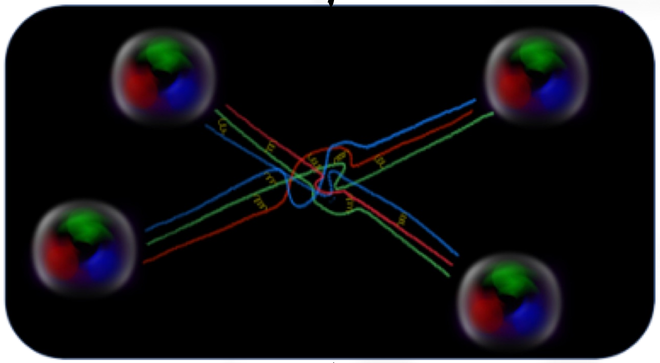
$$i = r,g,b \quad j = u,d,c,s,t,b$$

$$\mathcal{L}_{\rm EFT}\left[\pi, N, \ldots; m_{\pi}, m_{N}, \ldots; C_{i}\right]$$

C_i → LECs

LQCD + EFT

Absence of analytical solutions of QCD in the nonperturbative regime

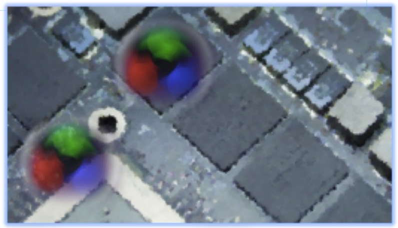


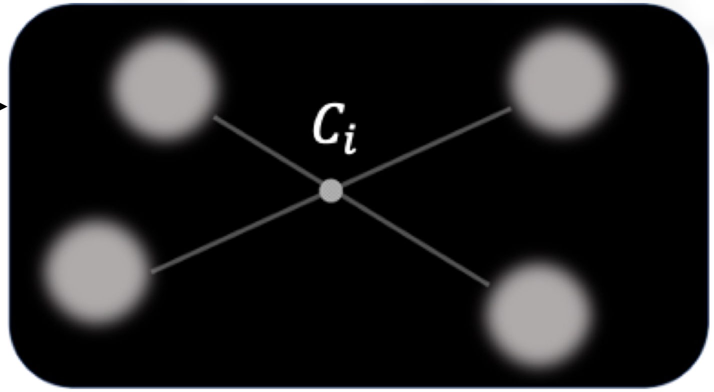
The quantum propagation is expressed as a weighted sum over paths

PATH INTEGRAL
Feynman, 1948

$$A = \int D(q)\, \exp\left(i \int_i^f dt\, L(q(t)) \right)$$

go to **Euclidean space**
(numerical methods/important sampling)





$$\mathcal{L}_{QCD} = \bar{q}_{ij}\left(i\gamma^{u}\partial_{u} - m_{j}\right)q_{ij} + g(\bar{q}_{ij}\gamma^{u}\lambda_{a}q_{ij})F_{u}^{a} - \frac{1}{4}F^{a}_{uv}F^{uv}_{a}$$

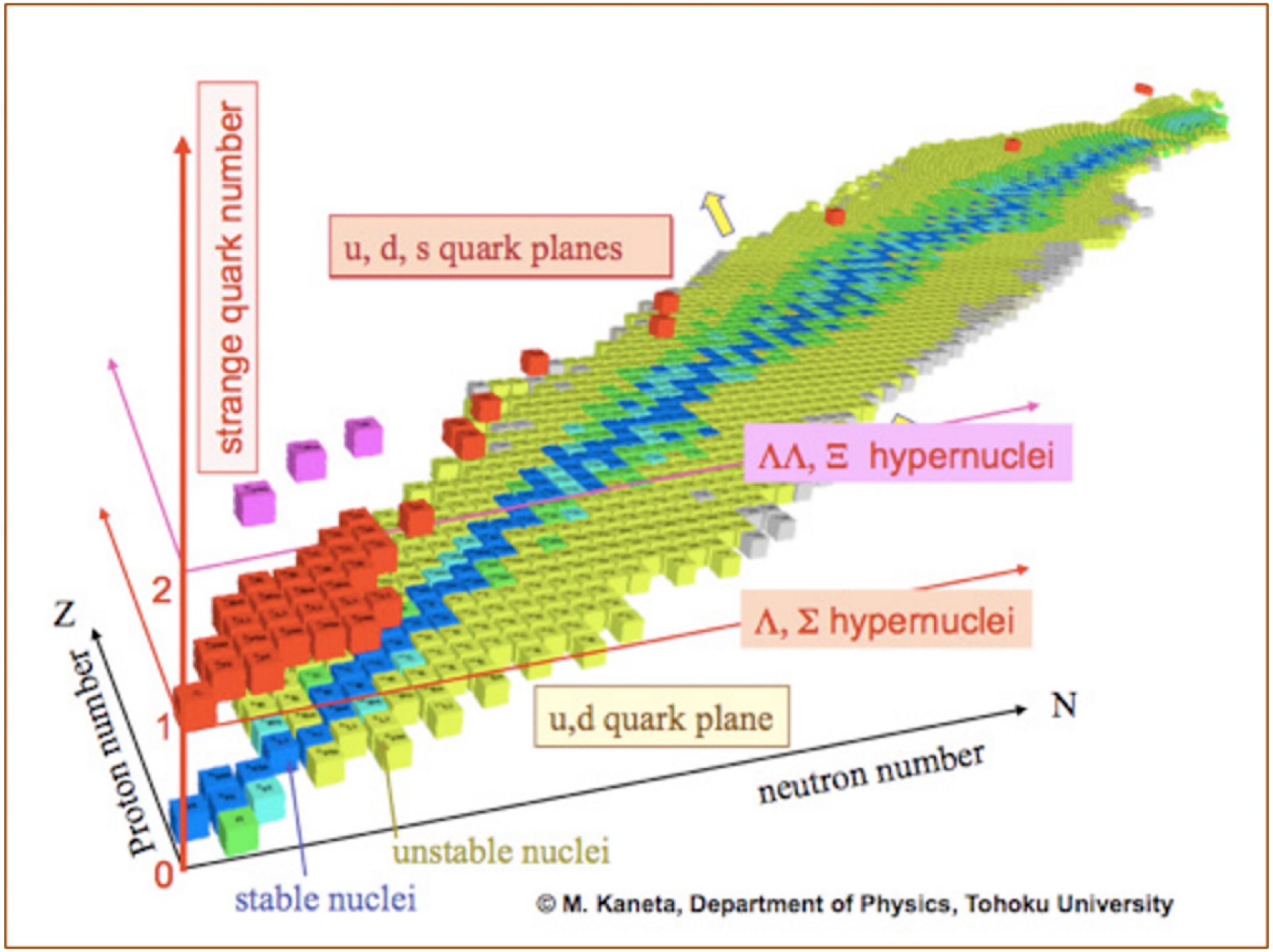
$$i = r,g,b \quad j = u,d,c,s,t,b$$

$$\mathcal{L}_{\mathrm{EFT}}\left[\pi, N, \ldots; m_\pi, m_N, \ldots; C_i\right]$$

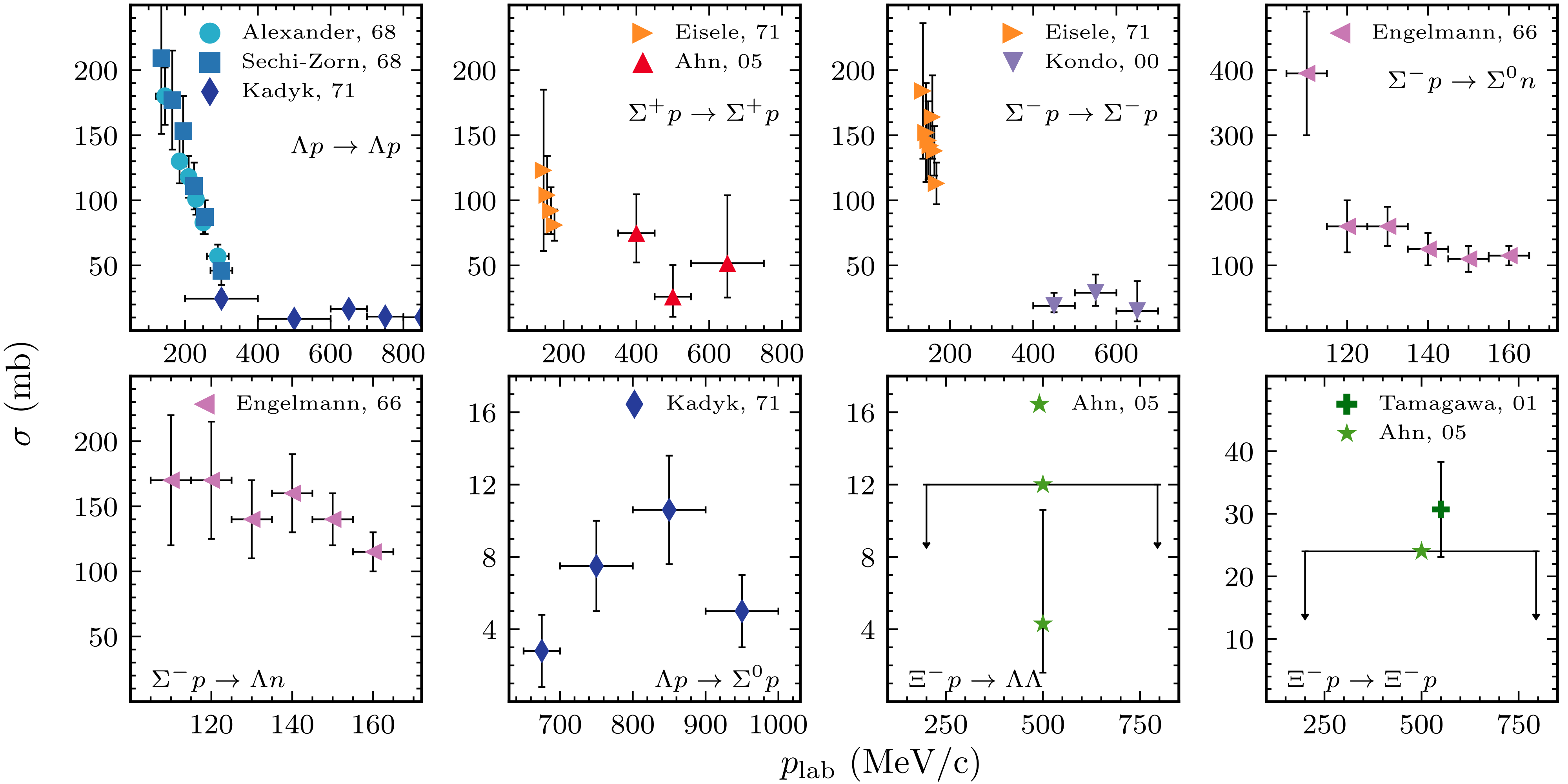
↳ LECs

STRANGE SECTOR

experimental information precluded by the instability of hyperons against the weak interaction



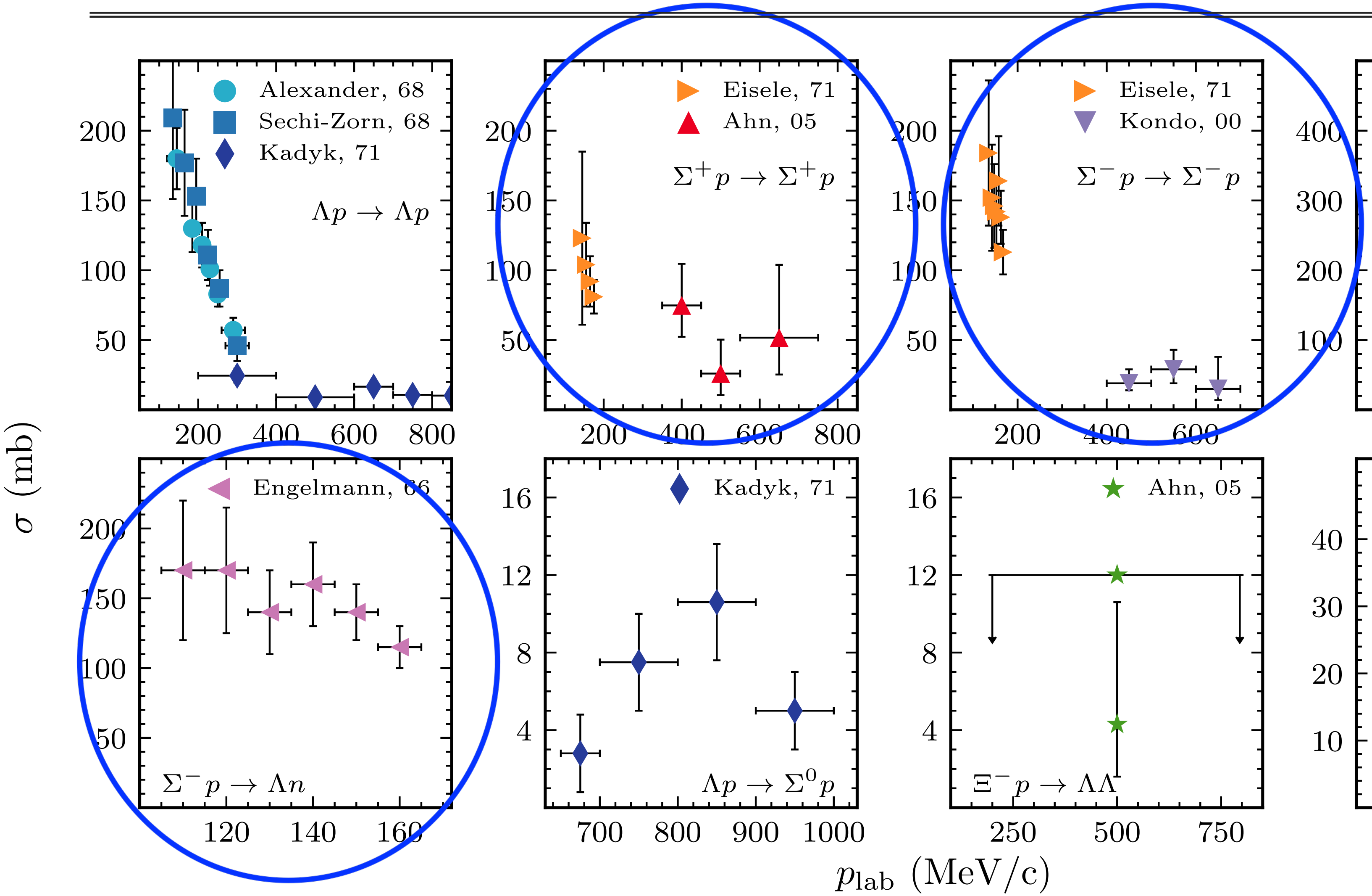
LQCD CALCULATIONS FOR NUCLEAR PHYSICS
PRACTICAL MOTIVATION



First collected in
Dover and Feschback,
Ann. Phys. 198 (1990)

updated by Marc Illa, IQuS, UW

LACK OF EXPERIMENTAL DATA IN THE STRANGENESS SECTOR. MOTIVATION



First collected in Dover and Feschback, Ann. Phys. 198 (1990)

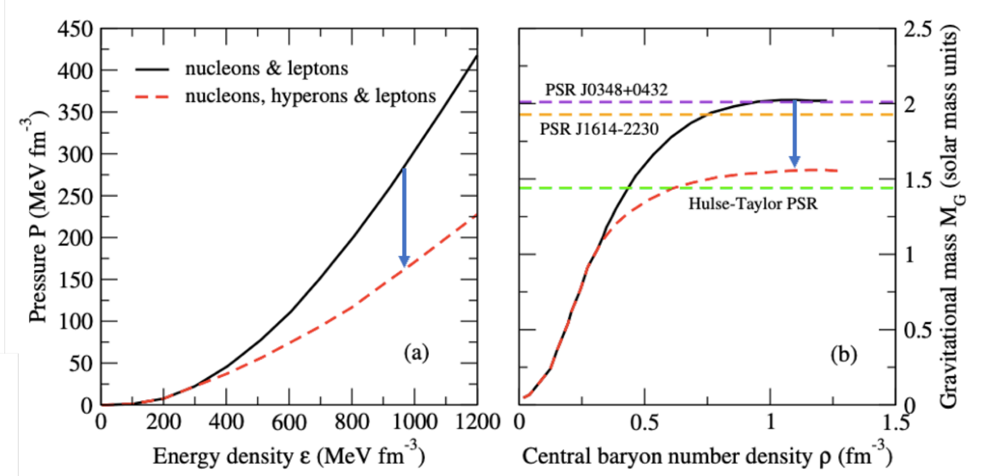
E40 @ JPARC

updated by Marc Illa, IQuS, UW

LACK OF EXPERIMENTAL DATA IN THE STRANGENESS SECTOR. SOME PHYSICAL IMPLICATIONS

Neutron Stars - Equation of State

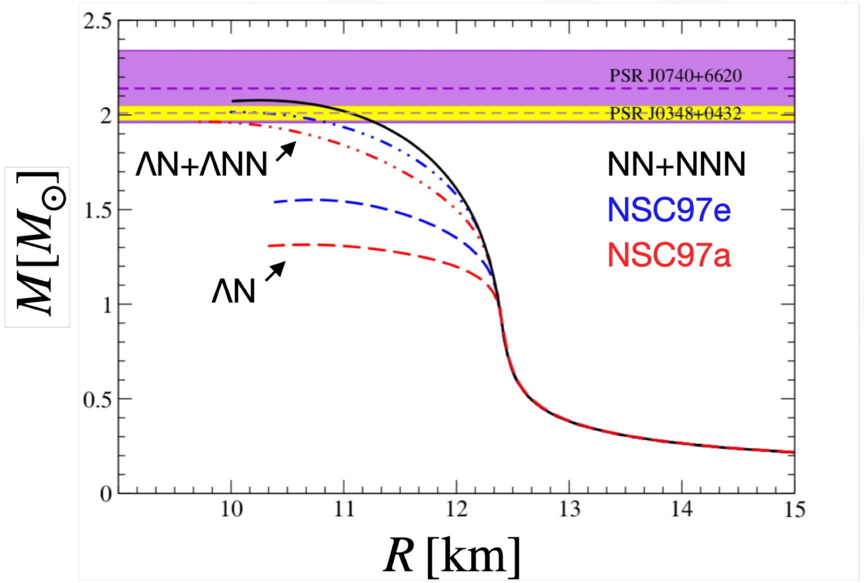
The composition of a neutron star depends on the hyperon properties in the medium (i.e. on the YN and YY interactions)



© Isaac Vidaña

Hyperons induce:

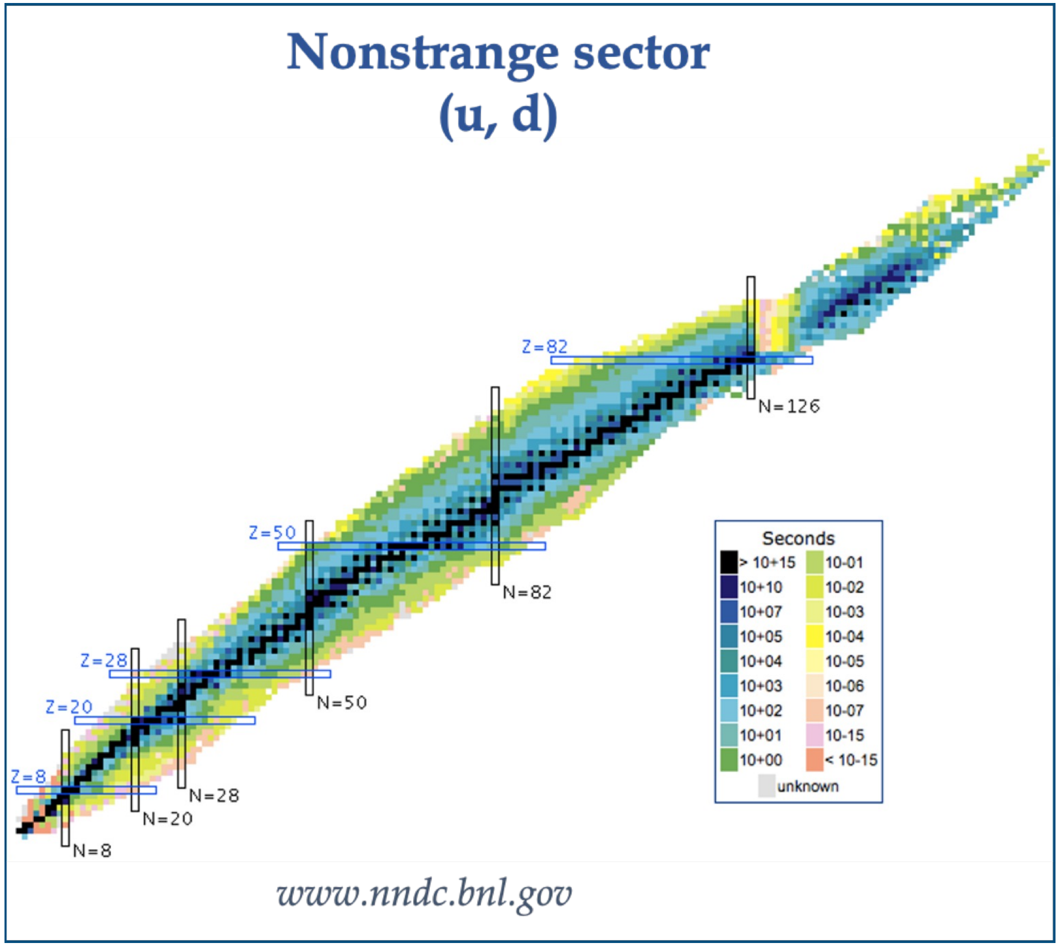
- softening of the EoS
- smaller M_{max}

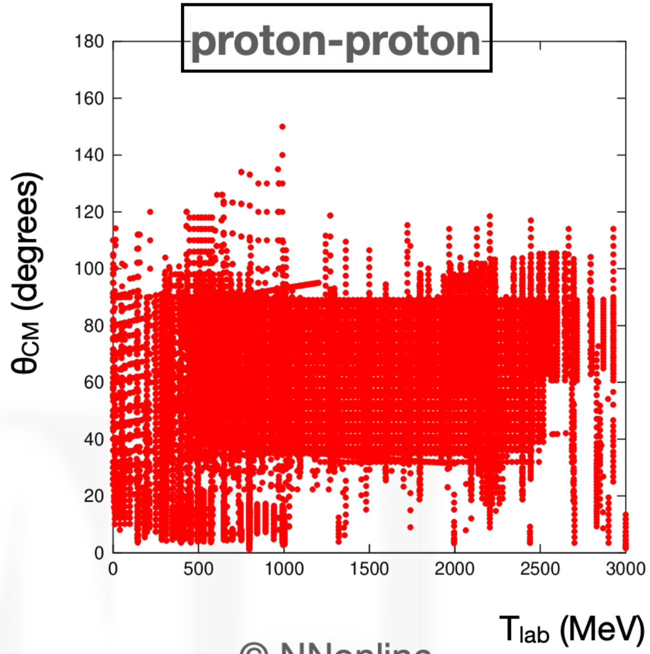


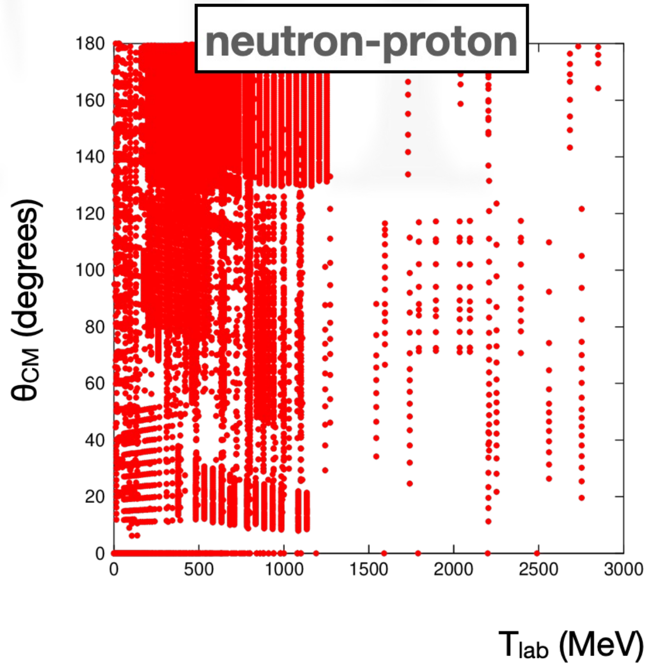
D. Logoteta, I. Vidaña, I. Bombaci, Eur. Phys. J.A 55 (2019)

Different models of the hyperon-nucleon interaction (constrained by experimental data) give different predictions

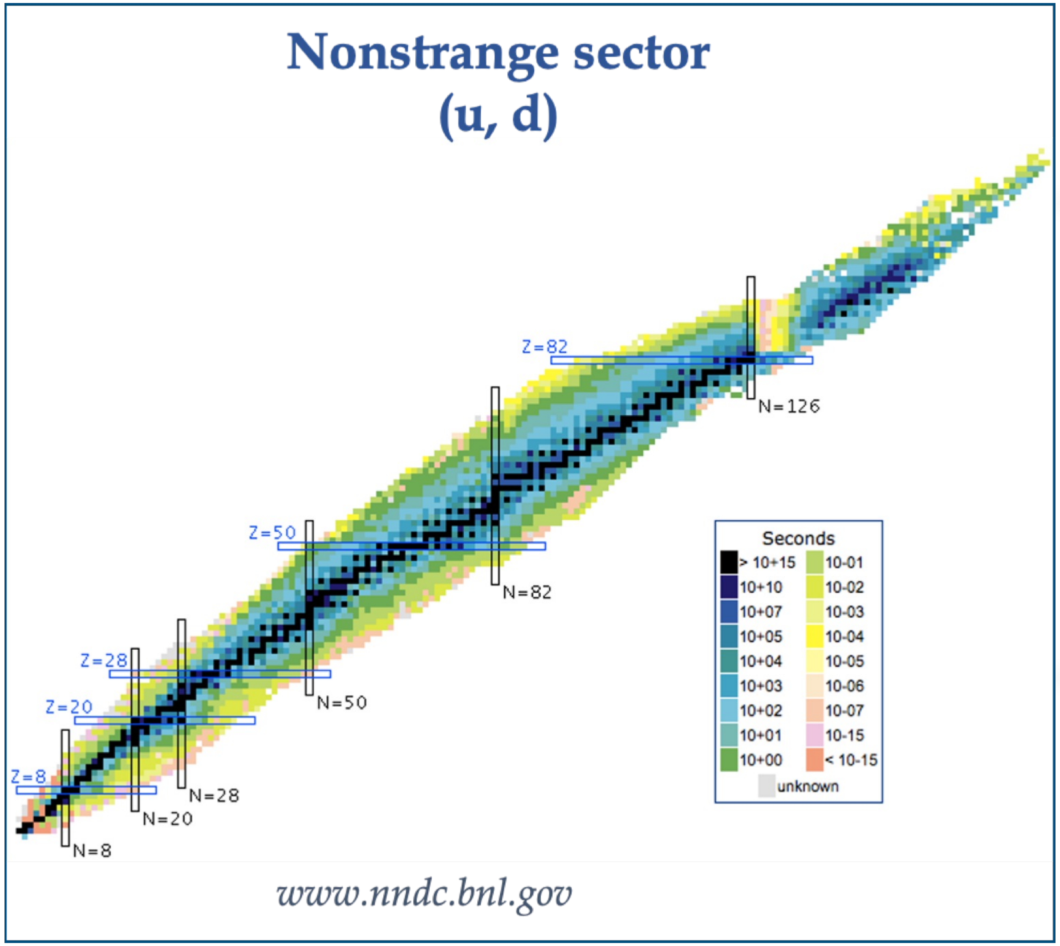
LQCD CALCULATIONS FOR NUCLEAR PHYSICS PRACTICAL MOTIVATION

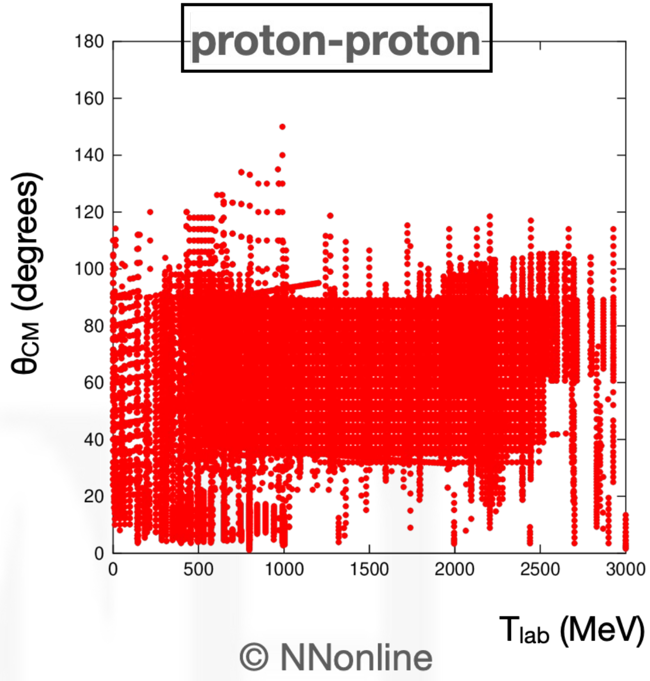


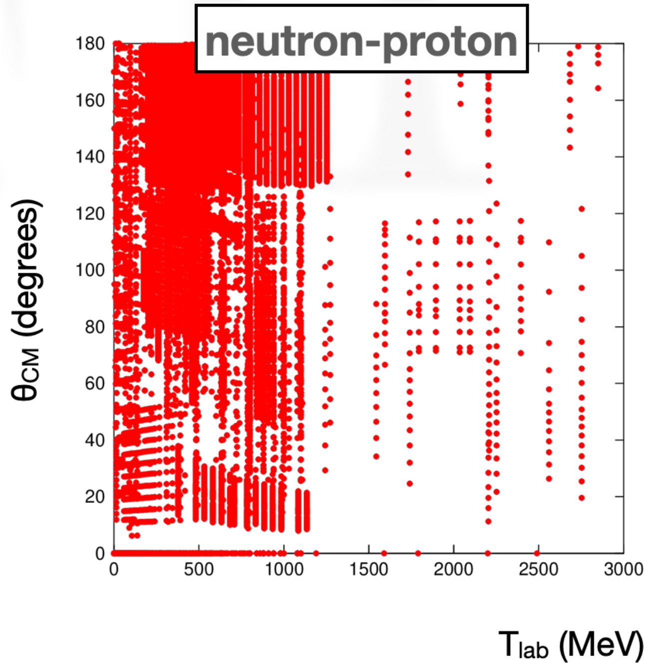




LQCD CALCULATIONS FOR NUCLEAR PHYSICS
PRACTICAL MOTIVATION







Lattice QCD allows us to make a direct connection to QCD

We can perform LQCD calculations with nucleons as a test of the method (by comparing with high-precision data)

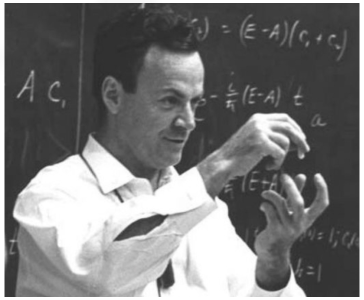
LQCD, a non-perturbative method

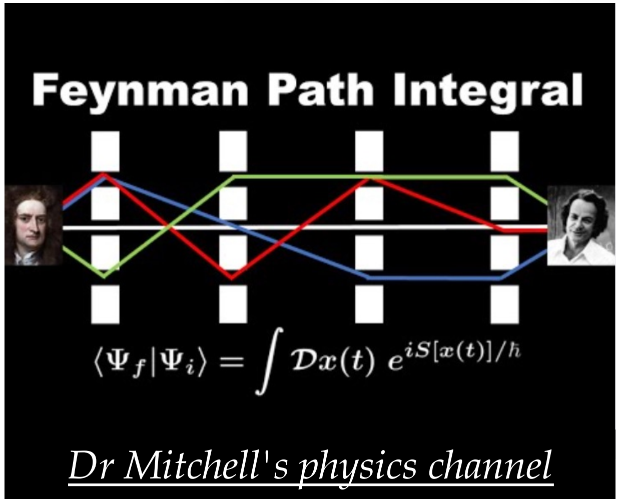
Lattice QCD provides us with a well-defined method to compute observables in the non-perturbative regime, implementing the Lagrangian of QCD. We intend to compute the theory on a computer, using methods analogous to those used in Statistical Mechanics.

These simulations allow us to compute correlation functions of hadronic operators, and matrix elements of any operator between hadronic states, in terms of the fundamental degrees of freedom of QCD

The method allows us to systematically improve the calculation and control the uncertainties

LQCD is a non-perturbative implementation of Field Theory, which uses the Feynman path-integral approach to evaluate transition matrix elements



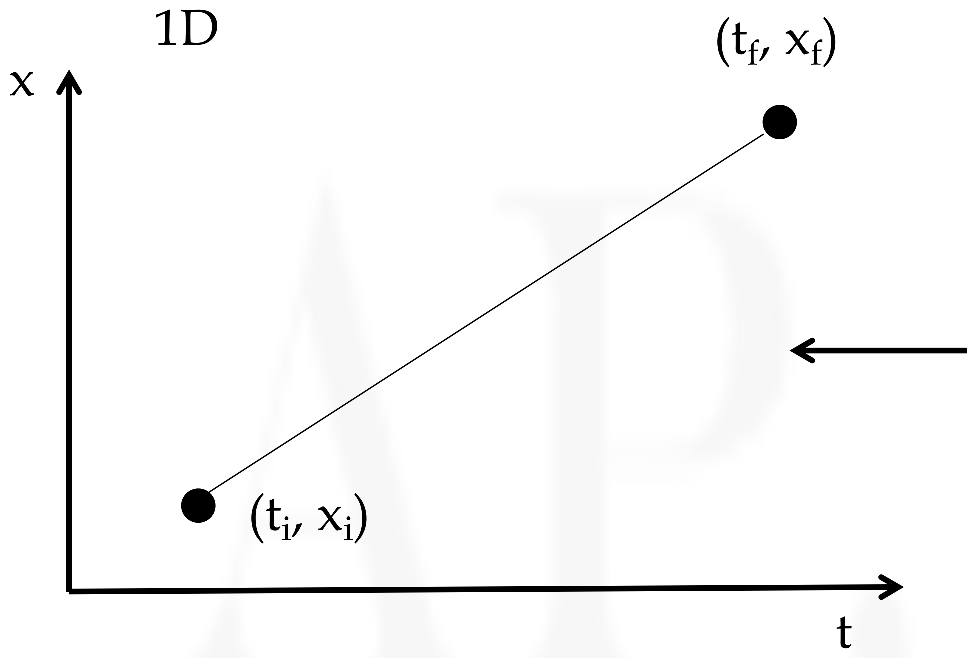


It replaces the classical notion of a single, unique trajectory for a system with a sum, or functional integral, over an infinity of possible trajectories to compute a quantum amplitude

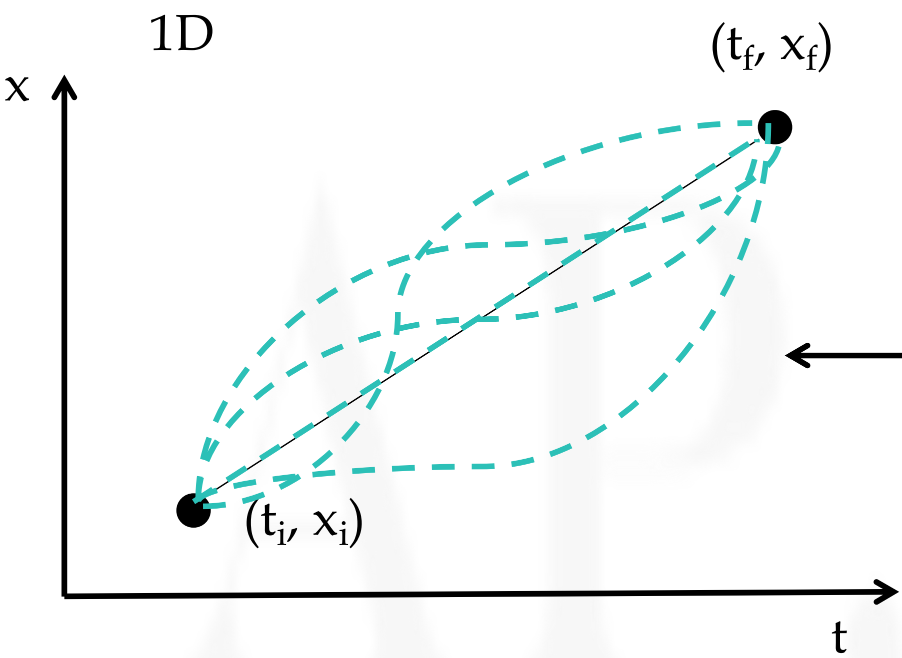
Study of the temporal evolution of particle states and of their interactions

$$\langle x_f, t_f | x_i, t_i \rangle = \langle x_f | e^{-iH(t_f - t_i)} | x_i \rangle$$

(1-D QM)

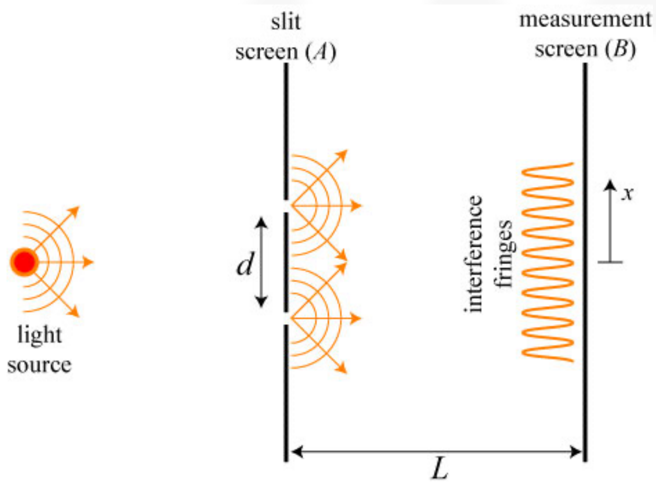


the classical path corresponds to the path with the minimum action

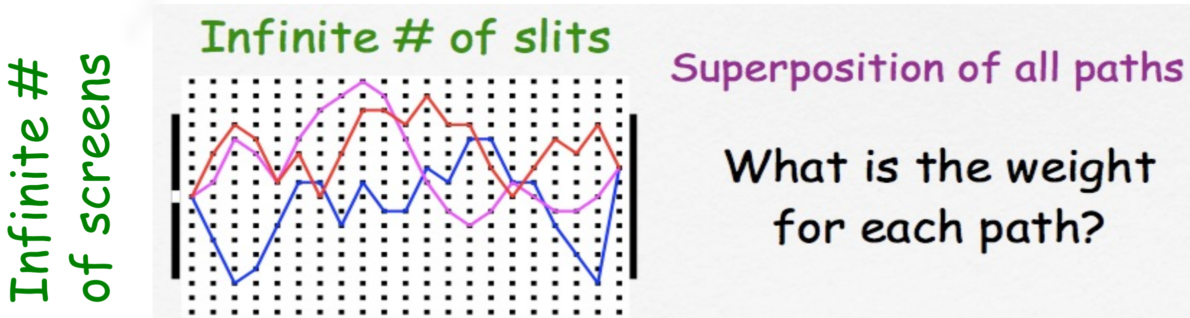


in quantum mechanics one sums over all possible paths

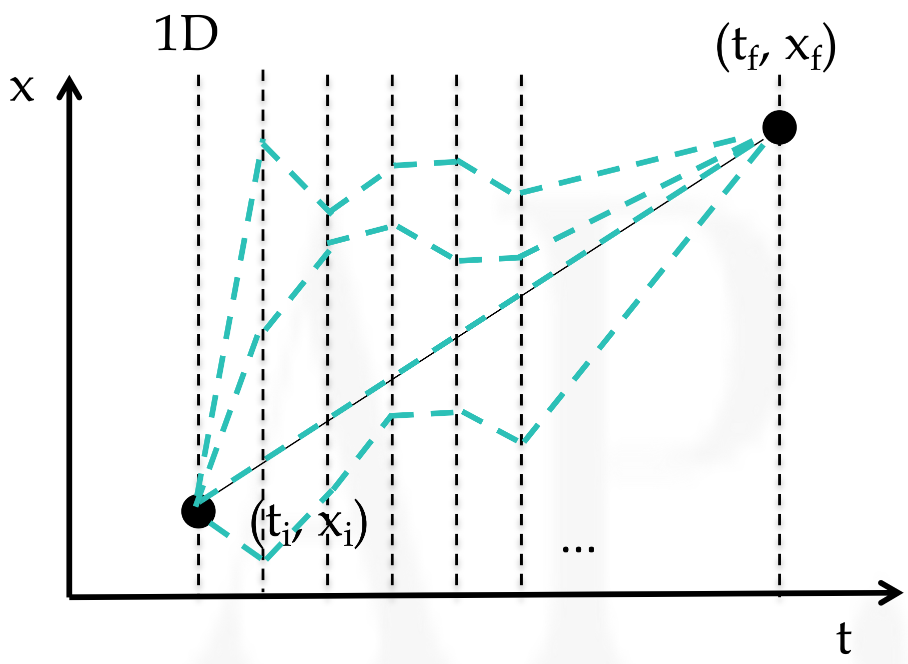
the classical path corresponds to the path with the minimum action



Young's double slit experiment



courtesy of Ross Young, Adelaide University



evolution of a quantum state
(1-D QM)

$$\langle x_f, t_f | x_i, t_i \rangle = \langle x_f | e^{-iH(t_f - t_i)} | x_i \rangle$$

$$\Delta t = (t_f - t_i)/N$$

$$\hat{1} = \int dx_i |x_i\rangle\langle x_i| \quad i = 1,2,....N-1$$

$$e^{-iHt} = e^{-iH\Delta t} \int dx_{N-1} |x_{N-1}\rangle\langle x_{N-1}| \; e^{-iH\Delta t} \int dx_{N-2} |x_{N-2}\rangle\langle x_{N-2}| \; \ldots \; e^{-iH\Delta t} \int dx_1 |x_1\rangle\langle x_1| e^{-iH\Delta t}$$

For an **interacting particle** with

$$\langle x_{k+1} | e^{-i\Delta t\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)} | x_k \rangle \xrightarrow{\Delta t \to 0} \int \frac{dp}{2\pi} \langle x_{k+1} | p \rangle e^{-i\Delta t \frac{p^2}{2m}} e^{-i\Delta t V(x_k)} \langle p | x_k \rangle$$

$$\langle x_{k+1}| e^{-i\Delta t\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)} |x_k\rangle \xrightarrow{\Delta t\to 0} \int \frac{dp}{2\pi}\langle x_{k+1}|p\rangle e^{-i\Delta t\frac{p^2}{2m}} e^{-i\Delta t V(x_k)}\langle p|x_k\rangle$$

$$\sim \int \frac{dp}{2\pi} e^{ip(x_{k+1}-x_k)} e^{-i\Delta t\frac{p^2}{2m}} e^{-i\Delta t V(x_k)} = \sqrt{\frac{2m\pi}{\Delta t}} e^{i\Delta t \sum_k \left[\frac{m}{2}\left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2 - V(x_k)\right]} + O(\Delta t^2)$$

$$\langle x_f, t_f | x_i, t_i\rangle = \langle x_f | e^{-iH(t_f-t_i)} | x_i\rangle \longrightarrow \int dx_{N-1}\int dx_{N-2}\cdots\int dx_1\, e^{i\Delta t \sum_k \left[\frac{m}{2}\left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2 - V(x_k)\right]}$$

$$\rightarrow \int_{x(0)=x_i}^{x(t)=x_f} D[x(t)]\, e^{iS_{classical}[x(t)]}$$

Lagrangian

RULE

each path, $q(t)$, contributes a phase given by the classical action

$$A_i \propto \exp\left(i\int_i^f dt\, L(q(t))\right)$$

The quantum propagation is expressed as a weighted sum over paths

Weight = complex phase factor given by the exponential of i times the classical action S

PATH INTEGRAL
Feynman, 1948

$$A = \int D(q)\, e^{i\int_i^f dt\, L(q(t))}$$

$$\langle x_{k+1}| e^{-i\Delta t\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)} |x_k\rangle \xrightarrow{\Delta t\to 0} \int \frac{dp}{2\pi} \langle x_{k+1}|p\rangle e^{-i\Delta t\frac{p^2}{2m}} e^{-i\Delta t V(x_k)} \langle p|x_k\rangle$$

$$\sim \int \frac{dp}{2\pi} e^{ip(x_{k+1}-x_k)} e^{-i\Delta t\frac{p^2}{2m}} e^{-i\Delta t V(x_k)} = \sqrt{\frac{2m\pi}{\Delta t}} e^{i\Delta t \sum_k \left[\frac{m}{2}\left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2 - V(x_k)\right]} + O(\Delta t^2)$$

$$\langle x_f, t_f | x_i, t_i\rangle = \langle x_f | e^{-iH(t_f-t_i)} | x_i\rangle = \int dx_{N-1} \int dx_{N-2} \cdots \int dx_1 \, e^{i\Delta t \sum_k \left[\frac{m}{2}\left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2 - V(x_k)\right]}$$

$$\to \int_{x(0)=x_i}^{x(t)=x_f} D[x(t)] e^{iS_{classical}[x(t)]}$$

Lagrangian

oscillating function
sign problem

Perform a Wick rotation: go from Minkowski to Euclidean space

PATH INTEGRAL
Feynman, 1948

$$A = \int D(q)\, e^{i\int_i^f dt\, L(q(t))}$$

By rotating to Euclidean time: $it \to \tau$

The propagation amplitude is re-expressed in terms of the Euclidean action, S_E

$$x_0 \equiv t \to -ix_4 \equiv -i\tau$$

$$p_0 \equiv E \to ip_4$$

$$x_E^2 = \sum_{i=1}^{4} x_i^2 = \vec{x}^2 - t^2 = -x_M^2$$

$$p_E^2 = \sum_{i=1}^{4} p_i^2 = \vec{p}^2 - E^2 = -p_M^2$$

$$i\Delta t \sum_k \left[\frac{m}{2} \left(\frac{x_{k+1} - x_k}{\Delta t} \right)^2 - V(x_k) \right]$$

Lagrangian

↓

$$-\Delta\tau \sum_k \left[\frac{m}{2} \left(\frac{x_{k+1} - x_k}{\Delta \tau} \right)^2 + V(x_k) \right]$$

Hamiltonian

By rotating to Euclidean time: $it \rightarrow \tau$

The propagation amplitude is re-expressed in terms of the Euclidean action, S_E

$$x_0 \equiv t \rightarrow -ix_4 \equiv -i\tau$$
$$p_0 \equiv E \rightarrow ip_4$$

$$x_E^2 = \sum_{i=1}^{4} x_i^2 = \vec{x}^2 - t^2 = -x_M^2$$
$$p_E^2 = \sum_{i=1}^{4} p_i^2 = \vec{p}^2 - E^2 = -p_M^2$$

$$i\Delta t \sum_k \left[\frac{m}{2}\left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2 - V(x_k) \right]$$

Lagrangian

$$-\Delta\tau \sum_k \left[\frac{m}{2}\left(\frac{x_{k+1}-x_k}{\Delta \tau}\right)^2 + V(x_k) \right]$$

Hamiltonian

$$e^{-\tau H} \rightarrow \int_{x(0)=x_i}^{x(t)=x_f} D[x_1, x_2, \ldots, x_{N-1}]\, e^{-\Delta\tau \sum_k \left[\frac{m}{2}\left(\frac{x_{k+1}-x_k}{\Delta \tau}\right)^2 + V(x_k) \right]}$$

The Euclidean path allows us to rewrite the oscillating phase as a decaying exponential

The weight of each path is a real positive quantity, looking like a ***Boltzmann factor***

BASIS OF NUMERICAL SIMULATIONS

Analogy with the partition function of a classical statistical mechanics system

Classical Statistical Mechanics	Euclidean Field Theory
$e^{-\frac{H}{kT}} \quad \rightarrow \quad Z = \sum_{conf} e^{-\frac{H(conf)}{kT}}$	$e^{-\frac{S}{h}} \quad \rightarrow \quad Z = \int D\phi \, e^{-\frac{S}{h}}$
$\langle \hat{O} \rangle$ canonical ensemble average	$\langle 0 \vert \hat{O} \vert 0 \rangle$ vacuum expectation value

Classical Statistical Mechanics

$$e^{-\frac{H}{kT}} \quad \rightarrow \quad Z = \sum_{conf} e^{-\frac{H(conf)}{kT}}$$

$\langle \hat{O} \rangle$ canonical ensemble average

$$\langle G[\phi] \rangle_T = \frac{\sum_{\phi} e^{-\frac{E[\phi]}{kT}} G[\phi]}{\sum_{\phi} e^{-\frac{E[\phi]}{kT}}}$$

~Thermal average over configurations

Euclidean Field Theory

$$e^{-\frac{S}{h}} \quad \rightarrow \quad Z = \int D\phi \, e^{-\frac{S}{h}}$$

$\langle 0 | \hat{O} | 0 \rangle$ vacuum expectation value

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{Z} \int \mathcal{D}q \mathcal{D}\bar{q} \mathcal{D}A_\mu \hat{\mathcal{O}}[q, \bar{q}, A] e^{-S_{QCD}^{(E)}[q,\bar{q},A]}$$

$\uparrow$

for ex. $\bar{u}(x_1)\gamma_5 d(x_1) \qquad \bar{d}(x_0)\gamma_5 u(x_0)$

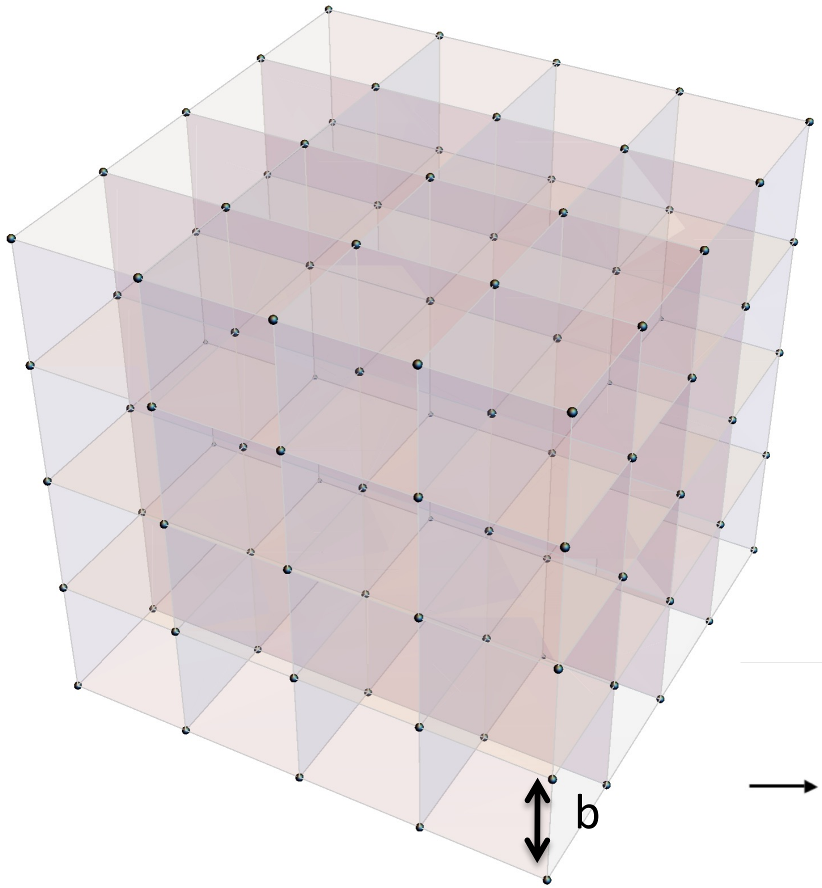
(for the calculation of the pion mass)

$L_x \times L_y \times L_z \times T \rightarrow (N_s \times N_s \times N_s) \times N_t$

$x = b\,(n_1, n_2, n_3, n_4) \qquad n_j \in \mathbb{Z}$

$$\vec{p} = \frac{2\pi}{L}\vec{n}, \quad n_\mu \in \mathbb{Z}$$

$$x_\mu = m_\mu b, \quad \text{with } m_\mu = 0,1,2,\ldots N-1, \quad \text{and } L = Nb$$

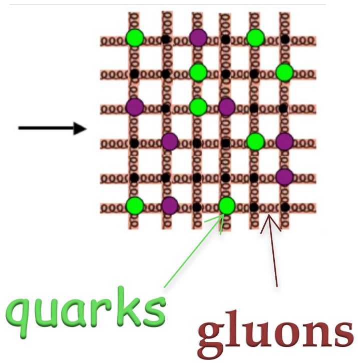


$$\Rightarrow p_{\max} = n_{\max}\frac{2\pi}{L} = \frac{N}{2}\frac{2\pi}{Nb} = \frac{\pi}{b}$$

cut-off

(largest wave vector)

$$\lambda_{\min} = 2b \quad \text{(shortest wave length)}$$



L >> relevant scales >> b

IR and UV cutoffs
(Euclidean spacetime)

Classical Statistical Mechanics	Euclidean Field Theory
$e^{-\frac{H}{kT}} \quad \rightarrow \quad Z = \sum_{conf} e^{-\frac{H(conf)}{kT}}$	$e^{-\frac{S}{h}} \quad \rightarrow \quad Z = \int D\phi \, e^{-\frac{S}{h}}$
$\langle \hat{O} \rangle$ canonical ensemble average	$\langle 0 \| \hat{O} \| 0 \rangle$ vacuum expectation value

In QCD the partition function in Euclidean space-time is:

$$Z = \int DA_\mu \, D\bar{\psi} \, D\psi \, \exp(-S_{QCD}) = \int DA_\mu \, D\bar{\psi} \, D\psi \, \exp\left(-\int d^4x \left(\frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a + \sum_f \bar{\psi}_f [D_\mu \gamma_\mu + m] \psi_f \right) \right)$$

Classical Statistical Mechanics

$$e^{-\frac{H}{kT}} \quad \rightarrow \quad Z = \sum_{conf} e^{-\frac{H(conf)}{kT}}$$

$\langle \hat{O} \rangle$ canonical ensemble average

Euclidean Field Theory

$$e^{-\frac{S}{h}} \quad \rightarrow \quad Z = \int D\phi \, e^{-\frac{S}{h}}$$

$\langle 0 | \hat{O} | 0 \rangle$ vacuum expectation value

In QCD the partition function in Euclidean space-time is:

$$Z = \int DA_\mu \, D\bar{\psi} \, D\psi \, \exp(-S_{QCD}) = \int DA_\mu \, D\bar{\psi} \, D\psi \, \exp\left(-\int d^4x \left(\frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a + \sum_f \bar{\psi}_f [D_\mu \gamma_\mu + m] \psi_f \right) \right)$$

gluons (8)

anti-quarks (6)

quarks (6)

$$DA_\mu \equiv \prod_x dA_\mu(x)$$

Classical Statistical Mechanics

$$e^{-\frac{H}{kT}} \quad \rightarrow \quad Z = \sum_{conf} e^{-\frac{H(conf)}{kT}}$$

$\langle \hat{O} \rangle$ canonical ensemble average

Euclidean Field Theory

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gluons (8)

anti-quarks (6)

quarks (6)

real, positive: will give us a weight → PROBABILITY

$$DA_\mu \equiv \prod_x dA_\mu(x)$$

Classical Statistical Mechanics	Euclidean Field Theory
$e^{-\frac{H}{kT}} \quad \rightarrow \quad Z = \sum_{conf} e^{-\frac{H(conf)}{kT}}$	$e^{-\frac{S}{h}} \quad \rightarrow \quad Z = \int D\phi \, e^{-\frac{S}{h}}$
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real, positive: will give us a weight → PROBABILITY

espin (4) x color (3)

$$DA_\mu \equiv \prod_x dA_\mu(x)$$

matter fields

ψ^{iaf} :

$i = 1,2,3,4$	Dirac index
$a = 1,2,3$	color index
$f = 1,2,\ldots n_f$	flavor index

Classical Statistical Mechanics

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gluons (8) — anti-quarks (6) — quarks (6)

$\exp(-S_{QCD})$: real, positive: will give us a weight → PROBABILITY

quarks, anti-quarks: espin (4) x color (3)

$$DA_\mu \equiv \prod_x dA_\mu(x)$$

functional integration

large # of degrees of freedom

matter fields

ψ^{iaf} :

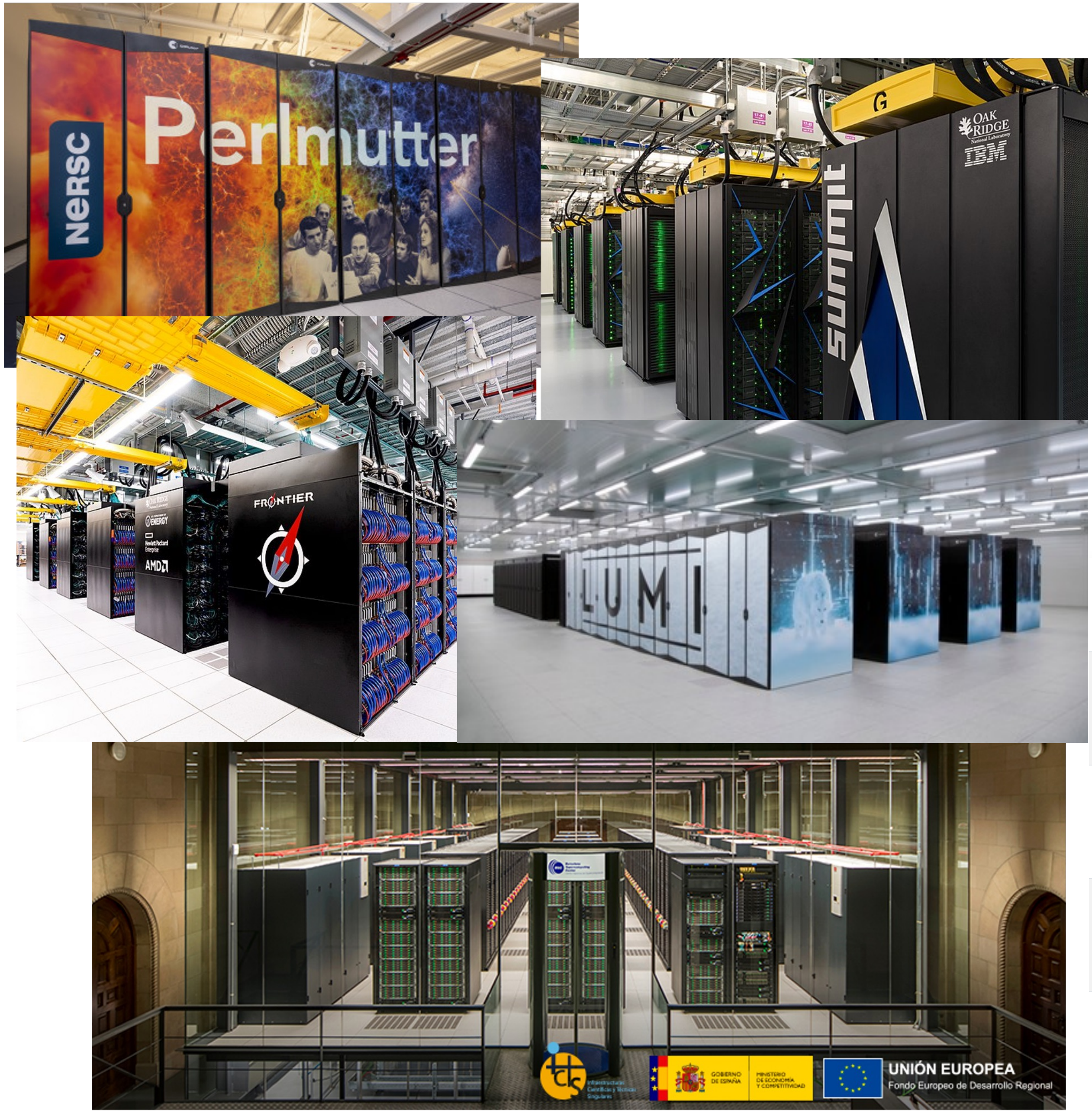
$i = 1,2,3,4$	Dirac index
$a = 1,2,3$	color index
$f = 1,2,\ldots n_f$	flavor index

dimension = 8 x 4 x 6 x 12 x 6 x 12 x # space points ~ 8 x 4 x 6 x 12 x 6 x 12 x 32^4 ~ 1.7 10^{11}

for $N_t = N_l = 32$

Requires the use of supercomputing facilities

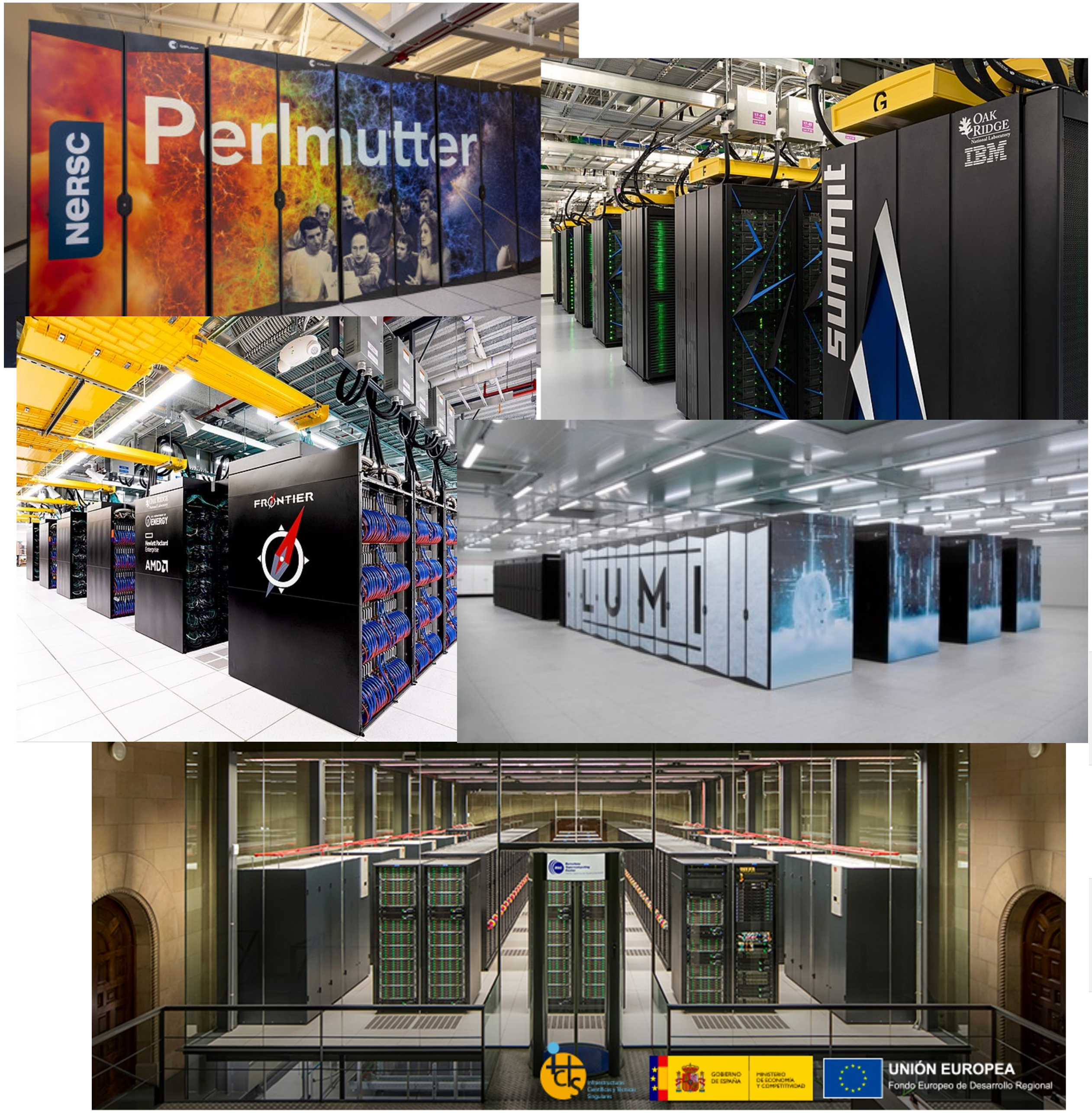
TOP500 The List. *June, 2024*



Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,206.00	1,714.81	22,786
2	**Aurora** - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States	9,264,128	1,012.00	1,980.01	38,698
3	**Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States	2,073,600	561.20	846.84	
4	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
5	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,752,704	379.70	531.51	7,107
6	**Alps** - HPE Cray EX254n, NVIDIA Grace 72C 3.1GHz, NVIDIA GH200 Superchip, Slingshot-11, HPE Swiss National Supercomputing Centre (CSCS) Switzerland	1,305,600	270.00	353.75	5,194
7	**Leonardo** - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN EuroHPC/CINECA Italy	1,824,768	241.20	306.31	7,494
8	**MareNostrum 5 ACC** - BullSequana XH3000, Xeon Platinum 8460Y+ 32C 2.3GHz, NVIDIA H100 64GB, Infiniband NDR, EVIDEN EuroHPC/BSC Spain	663,040	175.30	249.44	4,159
9	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148.60	200.79	10,096
10	**Eos NVIDIA DGX SuperPOD** - NVIDIA DGX H100, Xeon Platinum 8480C 56C 3.8GHz, NVIDIA H100, Infiniband NDR400, Nvidia NVIDIA Corporation United States	485,888	121.40	188.65	

Requires the use of supercomputing facilities

TOP 500 The List. *June, 2024*



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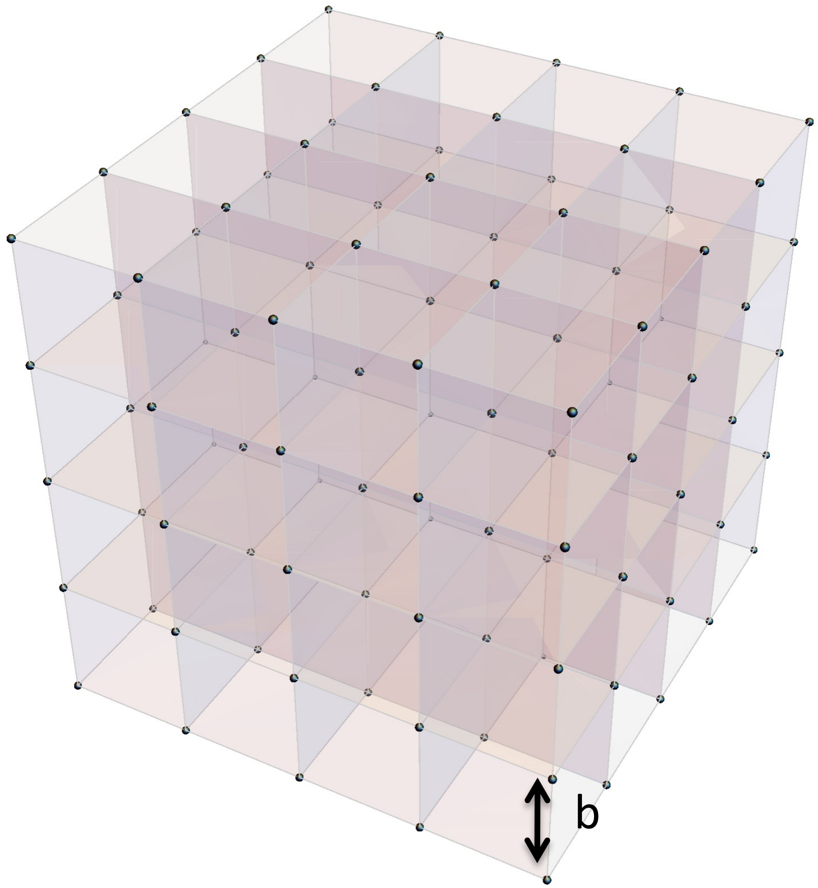
LQCD calculation, finite volume, discretization

$L_x \times L_y \times L_z \times T \ \rightarrow \ (N_s \times N_s \times N_s) \times N_t$

$x = b\,(n_1, n_2, n_3, n_4) \qquad n_j \in \mathbb{Z}$



$$\text{Cost} \approx \left[\frac{1}{m_q}\right] [L]^a \left[\frac{1}{b}\right]^\gamma$$

$L_x \times L_y \times L_z \times T \rightarrow (N_s \times N_s \times N_s) \times N_t$

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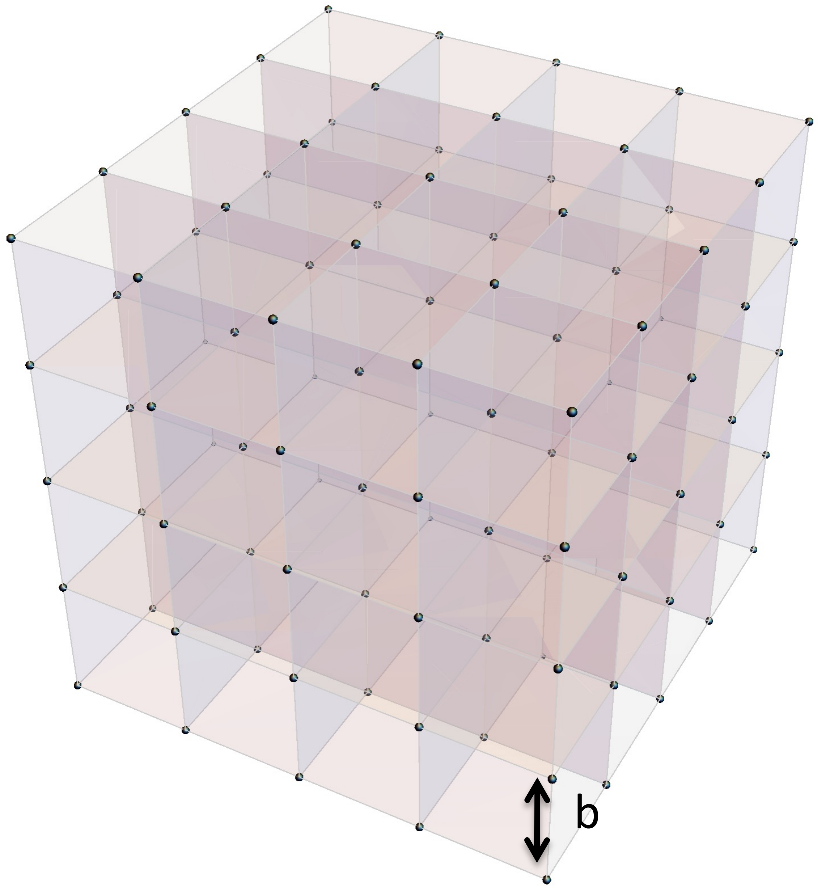


$$\text{Cost} \approx \left[\frac{1}{m_q}\right][L]^a\left[\frac{1}{b}\right]^\gamma$$

USE UNPHYSICAL VALUES FOR THESE PARAMETERS (LATTICE ARTIFACTS)

source of systematic errors in the numerical calculation

EFT Extrapolations

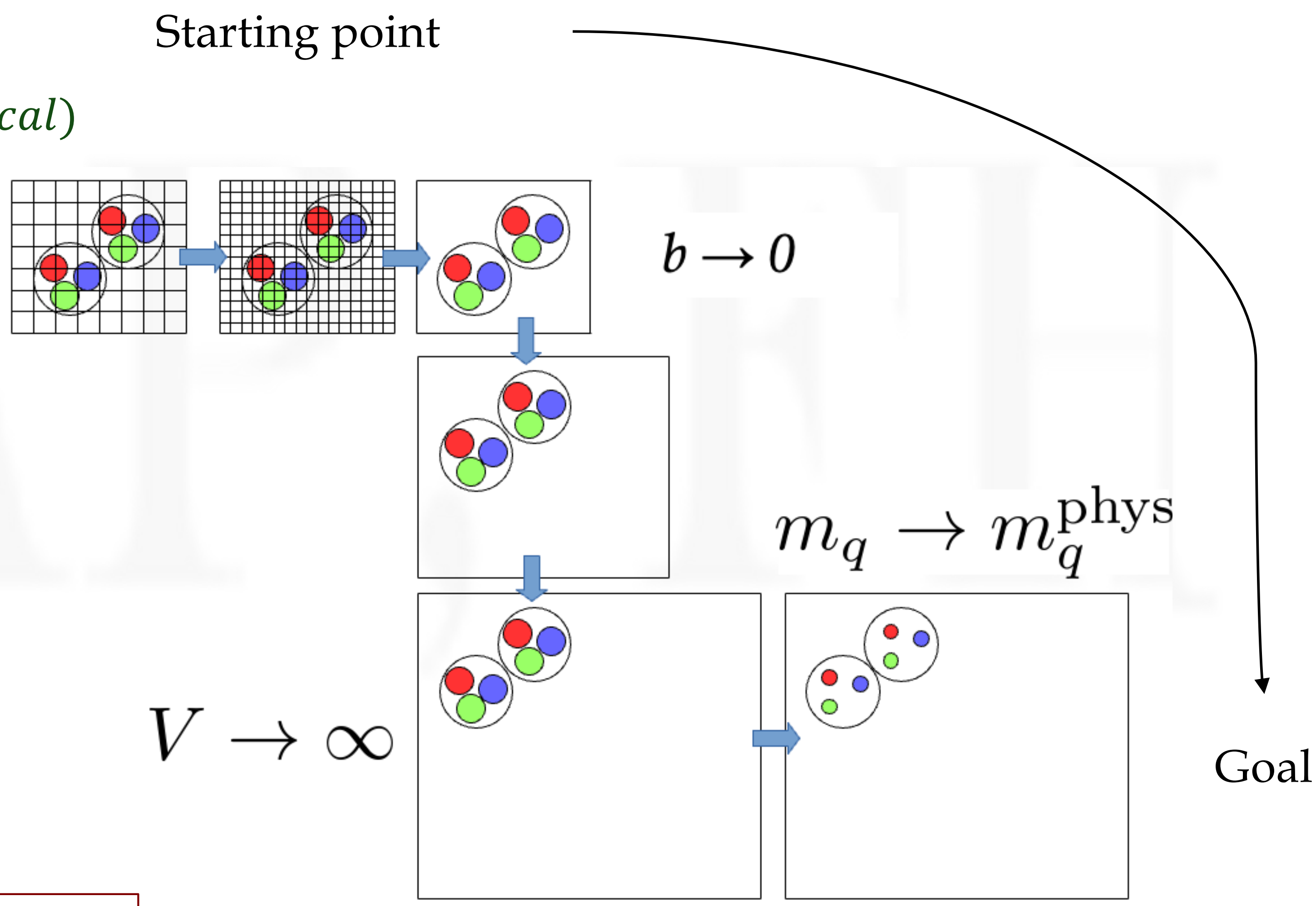
$L \rightarrow \infty$ $\qquad b \rightarrow 0$ $\qquad m_q \rightarrow m_q^{physical}$

LQCD calculation, finite volume, discretization

$L_x \times L_y \times L_z \times T$

b finite

$m_q > m_q$ (physical)



$$\text{Cost} \approx \left[\frac{1}{m_q}\right] [L]^a \left[\frac{1}{b}\right]^\gamma$$

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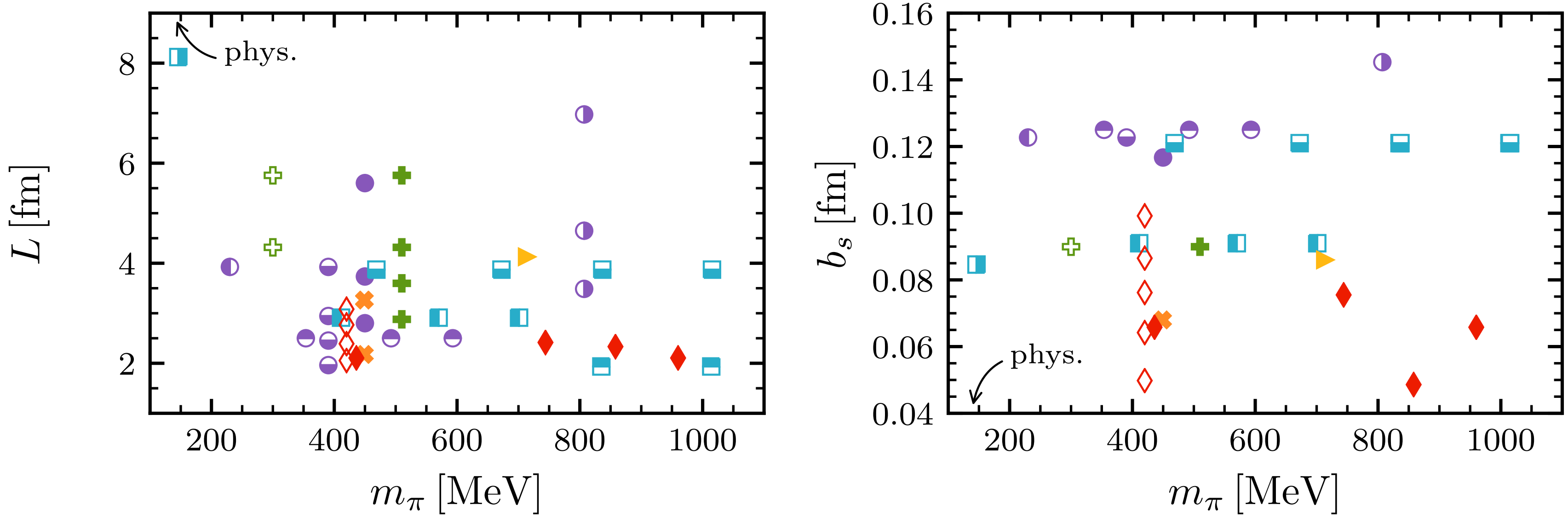
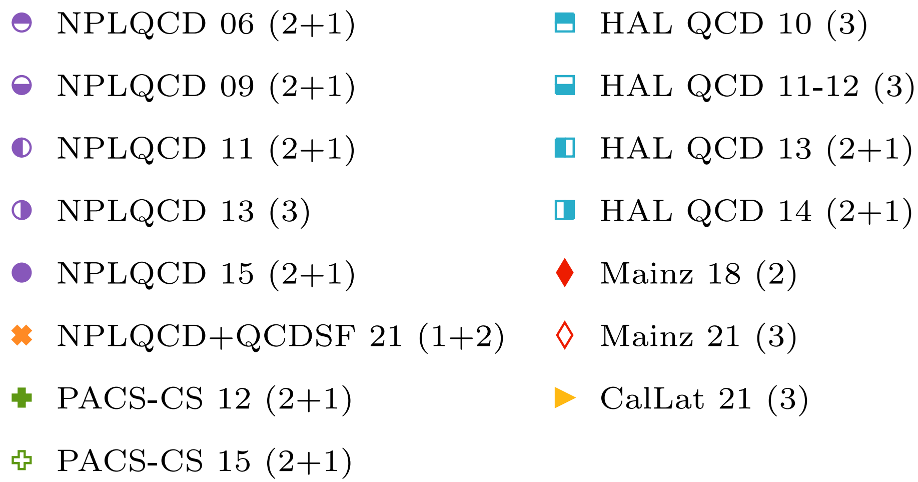
M. Illa, e-Print: 2109.10068 [hep-lat]



Collaborations



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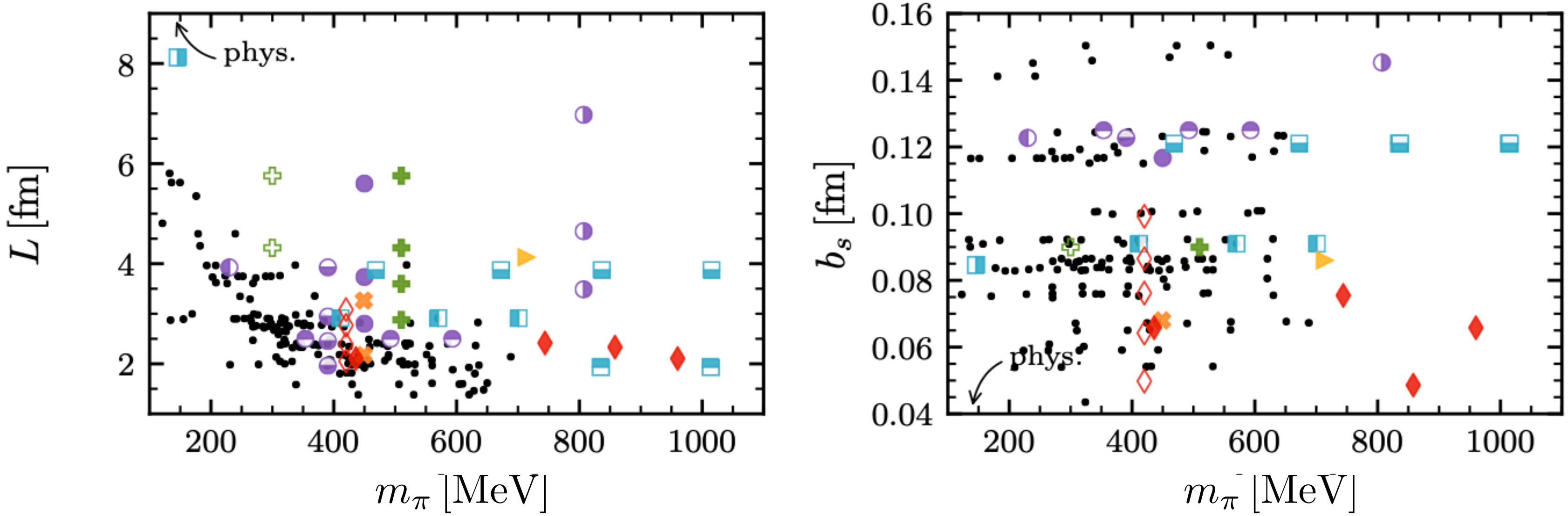
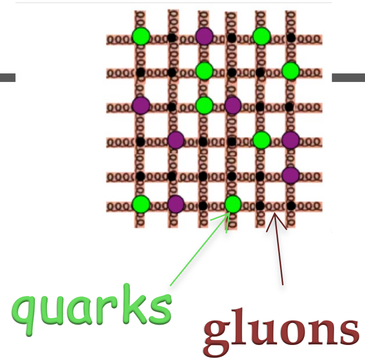


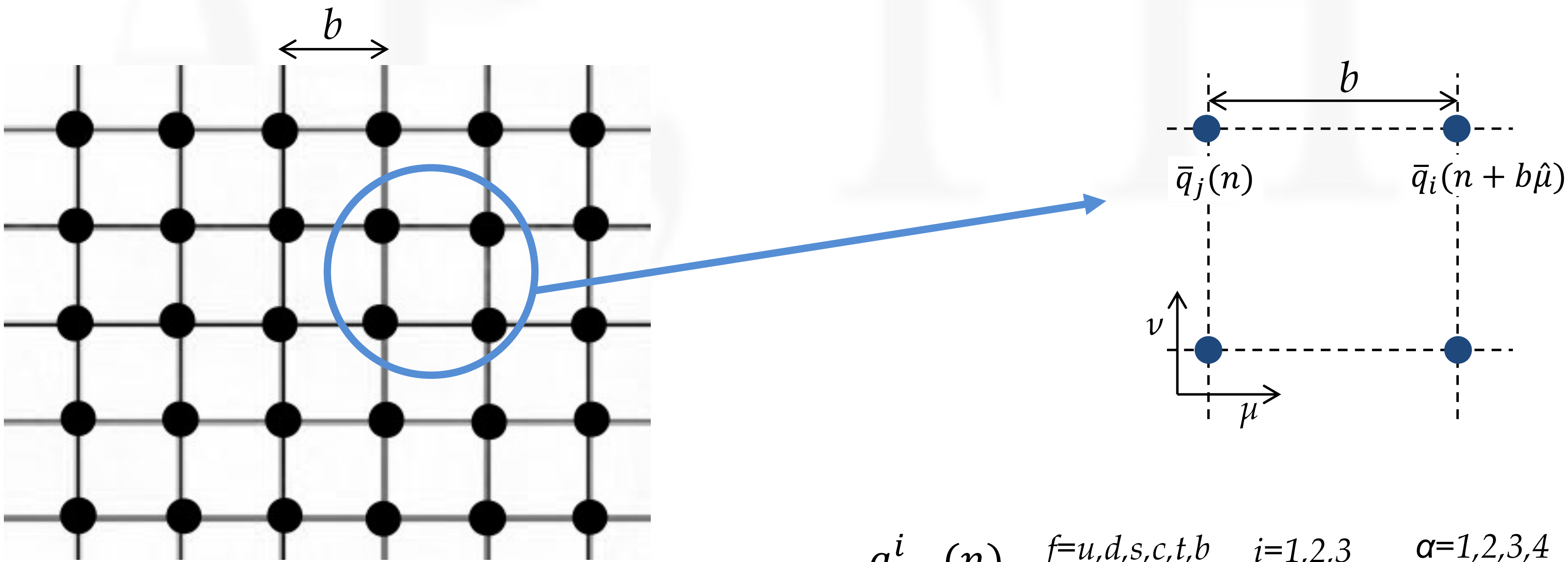
Collaborations

- NPLQCD 06 (2+1)
- NPLQCD 09 (2+1)
- NPLQCD 11 (2+1)
- NPLQCD 13 (3)
- NPLQCD 15 (2+1)
- NPLQCD+QCDSF 21 (1+2)
- PACS-CS 12 (2+1)
- PACS-CS 15 (2+1)
- HAL QCD 10 (3)
- HAL QCD 11-12 (3)
- HAL QCD 13 (2+1)
- HAL QCD 14 (2+1)
- Mainz 18 (2)
- Mainz 21 (3)
- CalLat 21 (3)
- • Single-hadron physics © C. Hoelbling

QCD on the computer



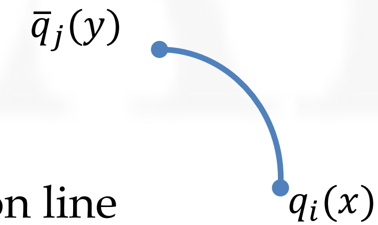
$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{Z} \int \mathcal{D}q\mathcal{D}\bar{q}\mathcal{D}A_\mu \hat{\mathcal{O}}[q,\bar{q},A] e^{-S^{(E)}_{QCD}[q,\bar{q},A]}$$



$q^i_{f,\alpha}(n)$ | f=u,d,s,c,t,b *flavor* | i=1,2,3 *color* | α=1,2,3,4 *Dirac*

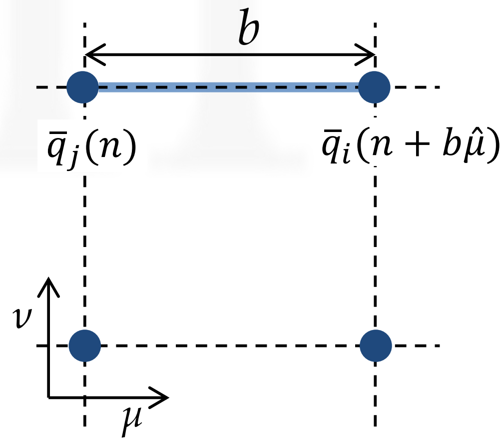
$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{Z} \int \mathcal{D}q \mathcal{D}\bar{q} \mathcal{D}A_\mu \hat{\mathcal{O}}[q, \bar{q}, A] e^{-S_{QCD}^{(E)}[q,\bar{q},A]}$$

continuum



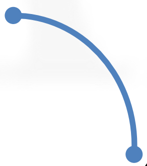
Wilson line

$$\bar{q}_j(y) \left[e^{ig \int_y^x dz_\mu A_\mu(z)} \right]_{ji} q_i(x)$$



$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{Z} \int \mathcal{D}q\mathcal{D}\bar{q}\mathcal{D}A_\mu \hat{\mathcal{O}}[q,\bar{q},A] e^{-S_{QCD}^{(E)}[q,\bar{q},A]}$$

continuum → lattice



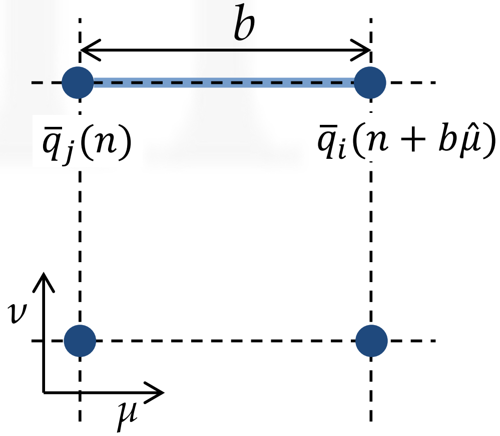
Wilson line

$$\bar{q}_j(y) \left[e^{ig\int_y^x dz_\mu A_\mu(z)} \right]_{ji} q_i(x)$$

$$\bar{q}_j(n) \left[e^{igbA_\mu(n)} \right]_{ji} q_i(n+b\hat{\mu})$$

define parallel transporters
or "links"

$$\bar{q}_j(n)\, U_\mu(n)\, q_i(n+b\hat{\mu})$$



$SU(3)_c$ matrices
with $\det U = 1,\ U^{-1} = U^\dagger$

Plaquette: smallest square (loop) on the lattice

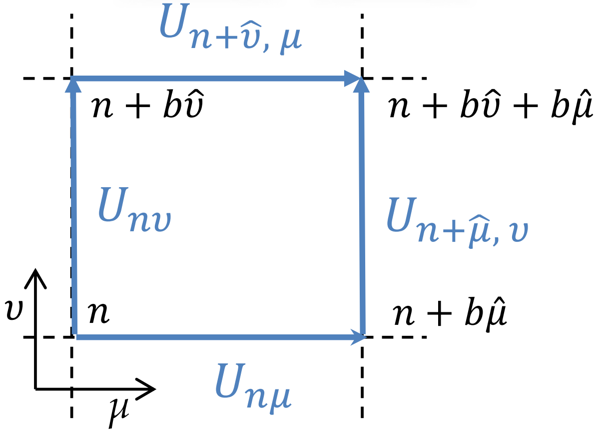
$$U_{n,\mu\upsilon} \equiv U_{n\mu} U_{n+\hat{\mu},\,\upsilon}\, U^{\dagger}_{n+\hat{\upsilon},\,\mu} U^{\dagger}_{n\upsilon}$$

Therefore, the gauge action will be written as $S[U] = \frac{\beta}{3} \sum_{n} \sum_{\mu<\upsilon} \Re\, \mathrm{Tr}\,(1 - U_{n,\mu\upsilon})$

$$\left(\beta = \frac{2N_c}{g^2}\right)$$

$$U_{n\mu} \equiv U_{\mu}(n) = \left[e^{igbA_{\mu}(n)}\right]$$

define parallel transporters
or “links”



What about the quarks?

Quark fields are Grasmann variables (anticommute)

Quark fields appear in the QCD action in a bilinear form: $S^F_{lattice} = \sum \bar{q}_f\, Q_f\, q_f$

$$Z = \int DA_\mu\, D\bar{\psi}\, D\psi\, \exp(-S_{QCD}) = \int DA_\mu\, D\bar{\psi}\, D\psi\, \exp\left(-\int d^4x \left(\frac{1}{4} G^a_{\mu\nu} G_a^{\mu\nu} - \sum_f \bar{\psi}_f [D_\mu \gamma_\mu + m] \psi_f\right)\right)$$

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The integral over the fermion fields gives us:

$$\int dq \, d\bar{q} \, e^{-\bar{q}Qq} = \det(Q)$$

$$\int dq \, d\bar{q} \, q(x) \, \bar{q}(y) \, e^{-\bar{q}Qq} = Q^{-1}_{xy} \det(Q)$$

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For example, the calculation of a quark propagator will be given by:

$$\langle q(x) \, \bar{q}(y) \rangle = \frac{1}{Z} \int dU \, dq \, d\bar{q} \, q(x) \, \bar{q}(y) \, e^{-\bar{q}Qq - S_G} = \frac{\int dU Q^{-1}_{xy} \det(Q) \;\; e^{-S_G}}{\int dU \det(Q) \;\; e^{-S_G}}$$

Note: *The quenched approximation consists in neglecting the effects of dynamical fermion loops in the path integral, i.e:* $\det(Q) = 1$

How do we write derivatives in discretized volume?

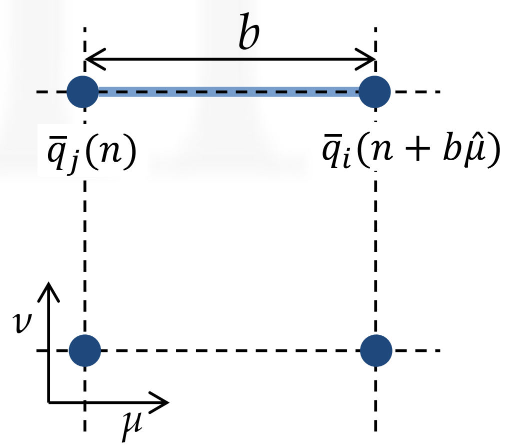
Basic discretized operators:

- Ordinary derivative: $$\partial_\mu q(x) \equiv \frac{1}{2b}[q(x+b\hat{\mu}) - q(x-b\hat{\mu})]$$

- Covariant derivative:

$$D_\mu q(x) \equiv \frac{1}{2b}\left[U_\mu(x) q(x+b\hat{\mu}) - U_{-\mu}(x) q(x-b\hat{\mu})\right]$$

("naive fermion action")



so that the discretized version is gauge invariant

Fermion doubling problem. Nielsen-Ninomiya theorem (Phys. Lett. 105B, 219 (1981))
"One cannot define lattice fermions having (standard) chiral symmetry without producing doublers"

Different strategies redifining the fermion action. Just to mention ...

Wilson fermions (*Phys. Rev. D10, 2445 (1974)*):

✓ add a term to the fermion action ~ $b\ \bar{q}\ \Delta\ q$ with Δ a covariant lattice Laplacian --> this gives a mass of the order *1/b* to the doublers (i.e. they decouple in the continuum limit ($b \rightarrow 0$)

✗ this term violates chiral symmetry
and introduces discretization errors linear in *b*
(can be eliminated by using $\mathcal{O}(b)$ − improved Wilson (clover)action, *Nucl. Phys. B259, 572 (1985)*)

Fermion doubling problem. Nielsen-Ninomiya theorem (Phys. Lett. 105B, 219 (1981))
"One cannot define lattice fermions having (standard) chiral symmetry without producing doublers"

Different strategies redifining the fermion action. Just to mention ...

Twisted-mass fermions (JHEP 08, 058 (2001)):
two flavors are treated together with an isospin-breaking mass term (the "twisted mass" term

✓ all errors linear in b are automatically removed by a clever choice of twisted mass and operators

✗ presence of isospin breaking effects

Staggered fermions (Phys. Rev. D16, 3031 (1977))

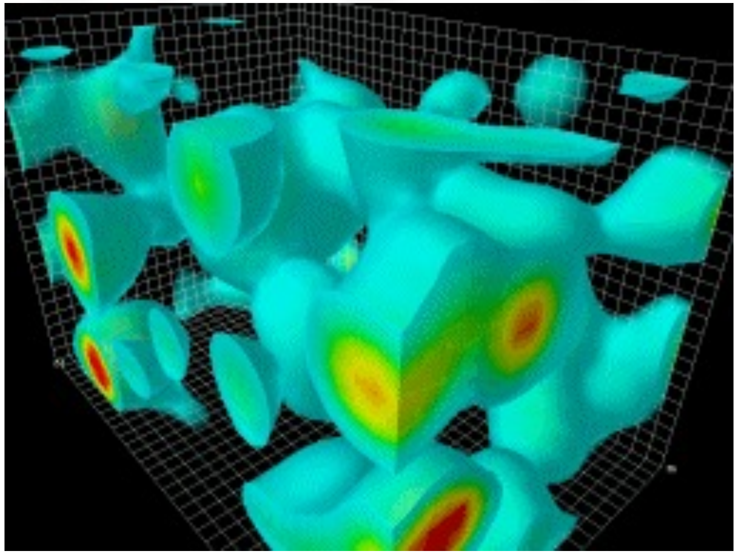
✓ faster to simulate than Wilson-like fermions
preserve some chiral symmetry
discretization errors of $O(b^2)$

✗ they retain some of the doublers (3 for d = 4: four degenerate fermions in the continuum limit)

Empty space is not empty. It's filled with the quark and gluon fields of QCD

Connecting to what we saw on path integrals...
Colour exchange by emission and absorption of gluons precisely describes path weighting
Paths of individual particles replaced by field configurations over all space

The QCD vacuum
This is a gluon field
This is what you would see when you stare into empty space if you could see gluons. The red hot spots indicate where the gluon field is strong. Isolated lumps correspond with the knotted-winding nature of the gluon field.



More animations:
https://sciences.adelaide.edu.au/physical-sciences/research/physics-research/cssm

$$Z = \int DU\; D\psi\; D\bar{\psi}\; e^{-\bar{\psi}Q(U)\psi - S_g[U]} = \int DU \left\{ \int D\psi\; D\bar{\psi}\; e^{-\bar{\psi}Q(U)\psi} \right\} e^{-S_g[U]}$$

$$= \int DU\, \det Q(U)\, e^{-S_g[U]}$$

$$\det\left[Q_f(A)\right] \equiv \det\left(\not{D}[A] + m\right)$$

(quark matrix)

LQCD algorithm

1. Generate an ensemble of N gauge-field configurations {U_i} according to the probability distribution P(U)

$$Z = \int DU\, D\psi\, D\bar{\psi}\, e^{-\bar{\psi}Q(U)\psi - S_g[U]} = \int DU \left\{ \int D\psi\, D\bar{\psi}\, e^{-\bar{\psi}Q(U)\psi} \right\} e^{-S_g[U]}$$

$$= \int DU \, \det Q(U)\, e^{-S_g[U]}$$

~ P(U)
Boltzmann weight

$$\det\left[Q_f(A)\right] \equiv \det\left(\not{D}[A] + m\right)$$

(quark matrix)

Time consuming task
(involves many local calculations)

$\left\{U^{[i]}\right\}$, (Markov process)

each configuration is created by the preceding one:

$$\mathrm{P}\left(U^{[i-1]} \to U^{[i]}\right) P\left(U^{[i-1]}\right) = \mathrm{P}\left(U^{[i]} \to U^{[i-1]}\right) P\left(U^{[i]}\right)$$

Basic Monte Carlo algorithm

1. Generate an ensemble of N gauge-field configurations $\{U_i\}$ according to the probability distribution P(U)

Monte Carlo production:

Start with an initial configuration U^0
- *cold: all links ~ identity*
- *hot: each link is a random SU(3) matrix*

Undertake an update process (the field value at each lattice site has to be updated) until it converges

$$\frac{P(U^{[i-1]} \to U^{[i]})}{P(U^{[i]} \to U^{[i-1]})} = e^{-\Delta S} \qquad \text{with} \qquad \Delta S = S(U^{[i]}) - S(U^{[i-1]})$$

A couple of examples of updating algorithms:

Metropolis: propose new random $U^{[i]}$ and accept/reject it with probability $P = \max(1, e^{-\Delta S})$
Heatbath: choose $U^{[i]}$ with probability $e^{-S(U^{[i]})}$ regardless of $U^{[i-1]}$

Reduce autocorrelations: use configurations separated t > auto-correlation length

LQCD algorithm

1. Generate an ensemble of N gauge-field configurations $\{U_i\}$ according to the probability distribution P(U)

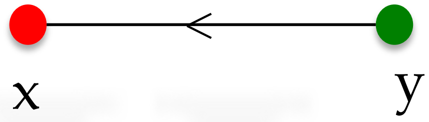
Once produced, configurations can be used for many different calculations.

There are collections of publicly available ensembles of configurations, with a range of values of lattice spacings, lattice sizes and quark masses.

Example, International Lattice Data Grid (ILDG)

https://hpc.desy.de/ildg/

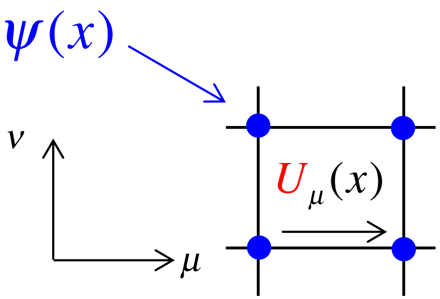
2. For each gauge-field configuration, calculate the quark propagator $Q^{-1}[U_i]$ (inverse of the fermion matrix, $\not{D}[A]+m$)



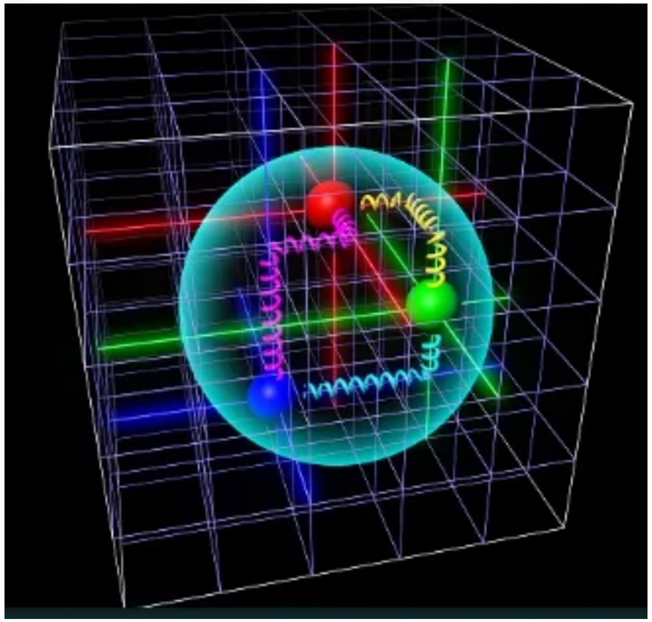
$$Q_u^{-1}(x,y) = u(y)\bar{u}(x)$$

$$\hat{O}\,[Q(U)^{-1}]$$

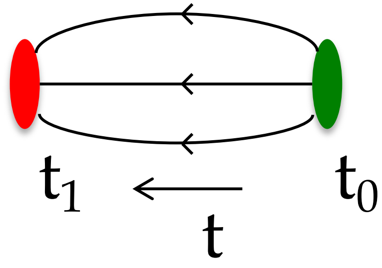
a large sparse matrix has to be inverted every time one needs an evaluation of the effective action



$$(U_{x\mu} \sim e^{igbA_{x\mu}})$$



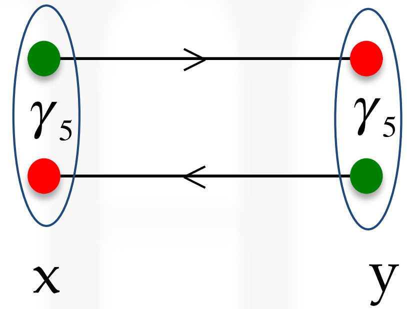
3. In order to study hadrons, we need to contract propagators onto correlation functions $C_i(t)$



$$C(\Gamma^\nu,\vec{p},t) = \sum_{\vec{x}_1} e^{-i\vec{p}\vec{x}_1}\, \Gamma^\nu \left\langle J(\vec{x}_1,t)\, \bar{J}(\vec{x}_0,0) \right\rangle$$

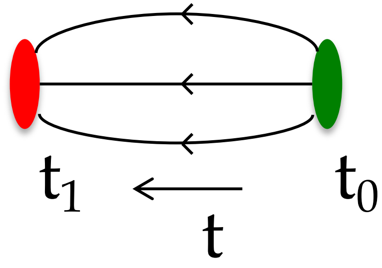
for ex. $\bar{u}(x_1)\gamma_5 d(x_1)$ $\bar{d}(x_0)\gamma_5 u(x_0)$

$\pi^+ = \bar{d}\gamma_5 u$



$$\left\langle \pi^\dagger(x)\, \pi(y) \right\rangle = \left\langle \bar{u}(x)\gamma_5 d(x)\, \bar{d}(y)\gamma_5 u(y) \right\rangle$$

3. In order to study hadrons, we need to contract propagators onto correlation functions $C_i(t)$



$$C(\Gamma^\nu,\vec{p},t)=\sum_{\vec{x}_1} e^{-i\vec{p}\vec{x}_1}\,\Gamma^\nu \left\langle J(\vec{x}_1,t)\bar{J}(\vec{x}_0,0)\right\rangle$$

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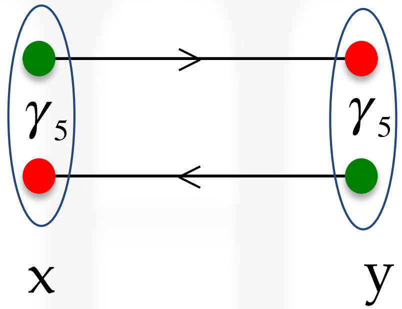
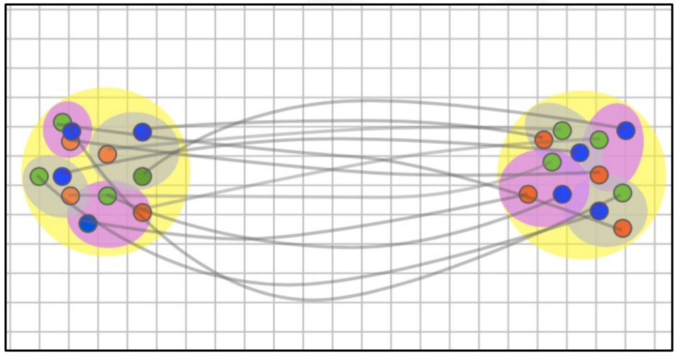


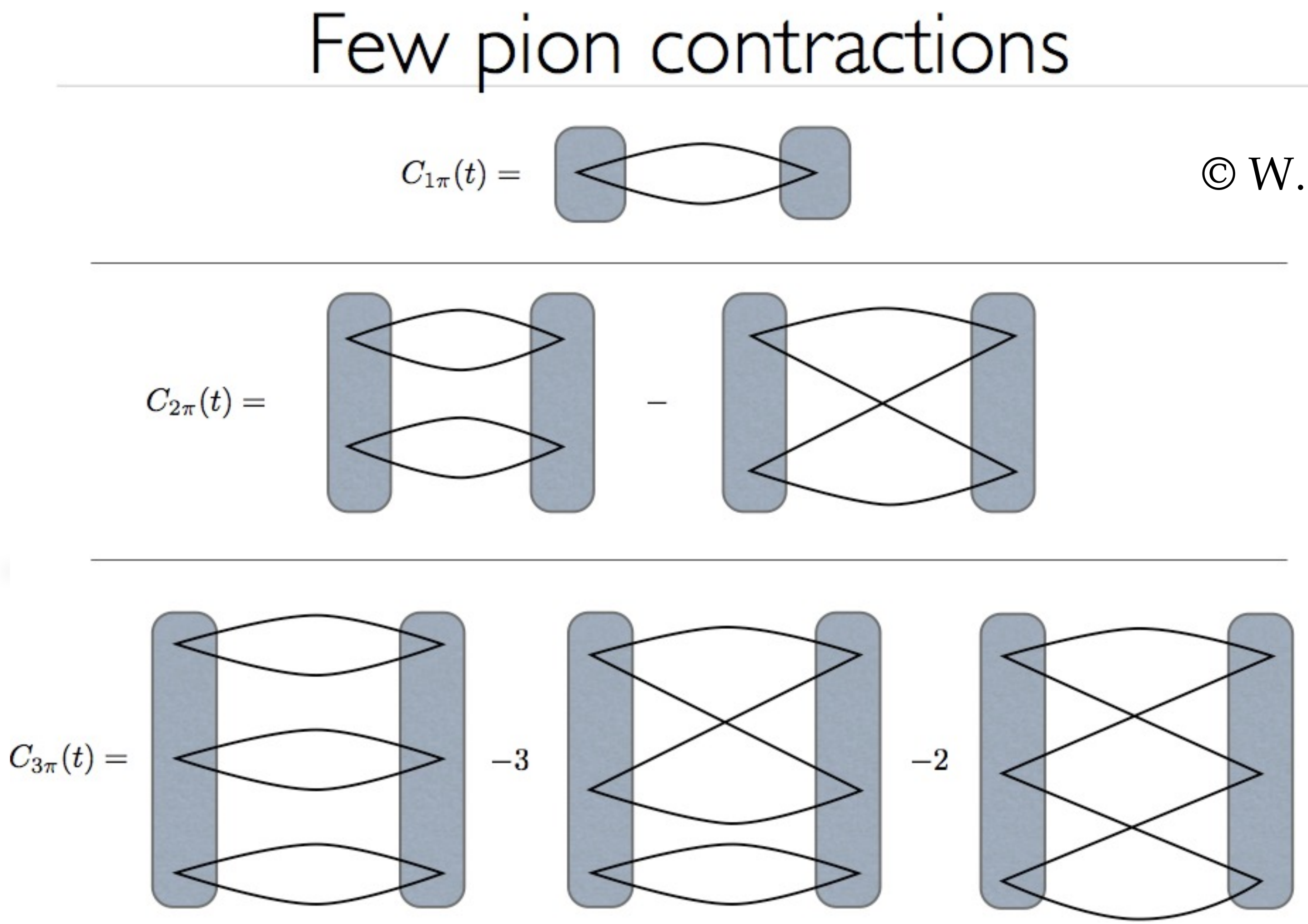
$$\left\langle \pi^\dagger(x)\,\pi(y)\right\rangle = \left\langle \bar{u}(x)\gamma_5 d(x)\,\bar{d}(y)\gamma_5 u(y)\right\rangle$$

Note: the number of Wick contractions increases rapidly with the number of hadrons



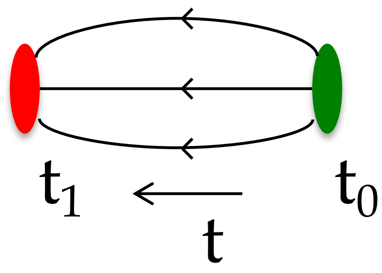
factorial growth in the number of contractions

increasing complexity of performing contractions with the number of hadrons
This is the real bootleneck for doing nuclear physics



© W. Detmold

3. In order to study hadrons, we need to contract propagators onto correlation functions C_i (t)

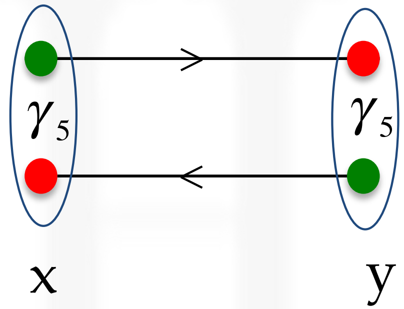


$$C(\Gamma^{\nu},\vec{p},t)=\sum_{\vec{x}_1} e^{-i\vec{p}\vec{x}_1}\,\Gamma^{\nu}\left\langle J(\vec{x}_1,t)\,\bar{J}(\vec{x}_0,0)\right\rangle$$

for ex. $\bar{u}(x_1)\gamma_5 d(x_1) \qquad \bar{d}(x_0)\gamma_5 u(x_0)$

Note: the number of Wick contractions increases rapidly with the number of hadrons

$$\pi^{+}=\bar{d}\gamma_5 u$$



$$\left\langle \pi^{\dagger}(x)\,\pi(y)\right\rangle=\left\langle \bar{u}(x)\gamma_5 d(x)\,\bar{d}(y)\gamma_5 u(y)\right\rangle$$

expectation values

$$\left\langle \hat{O}\right\rangle=\frac{1}{Z}\int DU\;D\bar{\psi}\;D\psi\,\hat{O}\,[\psi,\bar{\psi},U]\,e^{-\bar{\psi}Q(U)\psi-S_g[U]}$$

$$\left\langle \hat{O}\right\rangle=\frac{1}{Z}\int DU\;\underbrace{\hat{O}\,[Q(U)^{-1}]}_{\text{propagators}}\,\underbrace{\det(Q(U))\,e^{-S_g[U]}}_{\text{configurations }(\sim \text{P (U)})}$$

$$\xleftrightarrow[\lim N\to\infty]{}\;\left\langle \hat{O}\right\rangle=\frac{1}{N}\sum_{i=1}^{N}\hat{O}\,[Q(U_i)^{-1}]$$

gluon cfgs

$$\text{error}\sim\frac{1}{\sqrt{N}}$$

Example: *charged pion propagator* $\pi^+ = \bar{d}\gamma_5 u$

$$< \pi^{\dagger}(x)\pi(y) >=< \bar{u}(x)\gamma_5 d(x)\bar{d}(y)\gamma_5 u(y) >$$

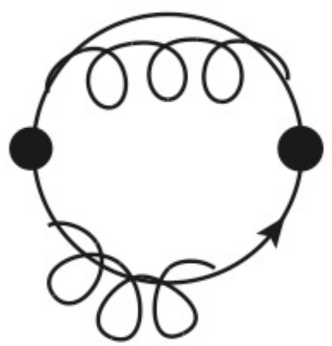
$$= \int \mathcal{D}U \mathcal{D}u \mathcal{D}\bar{u} \mathcal{D}d \mathcal{D}\bar{d} [\bar{u}\gamma_5 d\bar{d}\gamma_5 u] e^{\int(-\bar{u}G_u^{-1}u - \bar{d}G_d^{-1}d)+S_G} / Z$$

$$= \int \mathcal{D}U \det[G_u] \det[G_d] G_u(x,y)\gamma_5 G_d(y,x)\gamma_5 e^{-S_G} / Z$$

$$\Leftrightarrow < \pi^{\dagger}(x)\pi(y) >=< \bar{u}(x)\gamma_5 d(x)\bar{d}(y)\gamma_5 u(y) > .$$

$G_u(y,x) = u(x)\bar{u}(y)$

Wick contractions
(equivalent to the path integral)



$$< \pi^{+}(x)\pi(y) >=< Tr[G_u(x,y)\gamma_5 G_d(y,x)\gamma_5] >$$

(connected quark diagram)

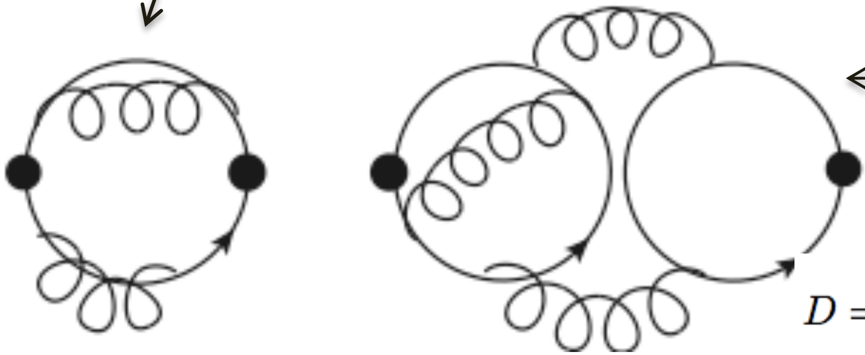
Example: *neutral pion propagator*

$$\pi^0 = \frac{\bar{u}u + \bar{d}d}{\sqrt{2}}$$

$$G_u(y,x) = u(x)\bar{u}(y)$$

$$
\begin{aligned}
<\pi^\dagger(x)\pi(y)> &= <\frac{1}{2}(\bar{u}(x)u(x) + \bar{d}(x)d(x))(\bar{u}(y)u(y) + \bar{d}(y)d(y))> \\
&= \frac{1}{2}[<\bar{u}(x)u(x)\bar{u}(y)u(y)> + <\bar{d}(x)d(x)\bar{d}(y)d(y)> \\
&\quad + <\bar{d}(x)d(x)\bar{u}(y)u(y)> + <\bar{u}(x)u(x)\bar{d}(y)d(y)>] \\
&= \frac{1}{2}[<\bar{u}(x)u(x)\bar{u}(y)u(y)> + <\bar{d}(x)d(x)\bar{d}(y)d(y)> \\
&\quad + <\bar{u}(x)u(x)\bar{u}(y)u(y)> + <\bar{d}(x)d(x)\bar{d}(y)d(y)> \\
&\quad + <\bar{d}(x)d(x)\bar{u}(y)u(y)> + <\bar{u}(x)u(x)\bar{d}(y)d(y)>] .
\end{aligned}
$$

$$<\pi^+(x)\pi(y)> = <Tr[G_u(x,y)\gamma_5 G_d(y,x)\gamma_5]>$$



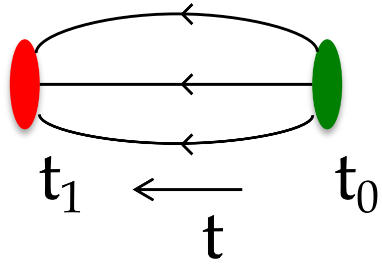
$$G_d(x,y) = \gamma_5 G_u^+(y,x)\gamma_5$$

$$D = \frac{1}{2} <Tr[G_u + G_u^+]Tr[G_u + G_u^+]> = 2 <(Tr[Re(G_u)])^2>$$

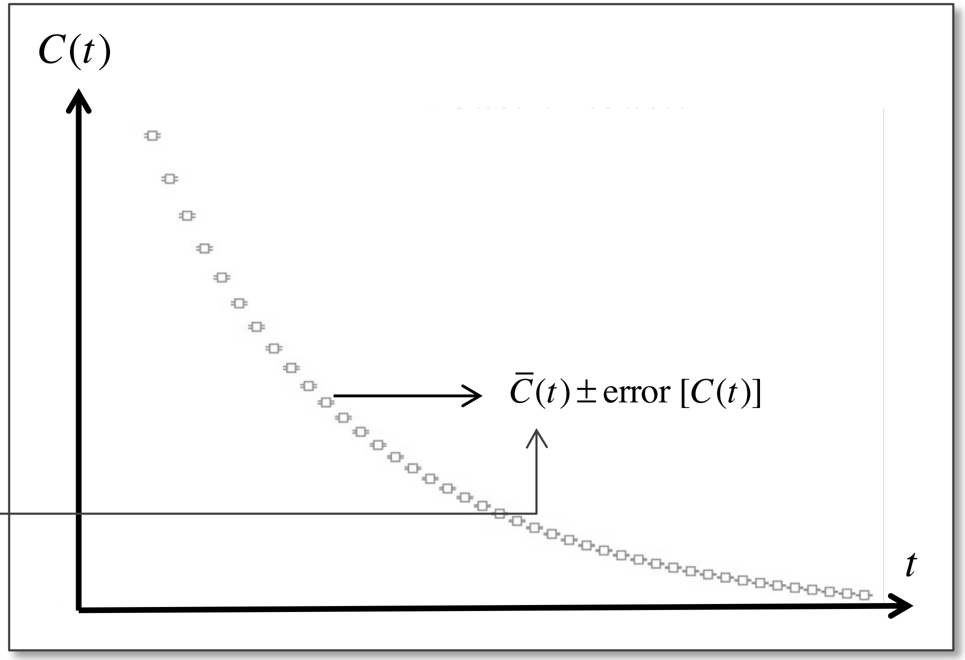
(connected and disconnected quark diagrams)

correlation functions $C_i(t)$

$$C(\Gamma^\nu,\vec{p},t)=\sum_{\vec{x}_1} e^{-i\vec{p}\vec{x}_1}\,\Gamma^\nu\left\langle J(\vec{x}_1,t)\bar{J}(\vec{x}_0,0)\right\rangle$$



average over N gauge-field configurations $\{U_{x\mu}\}^i$ with $i=1,2,\ldots N$



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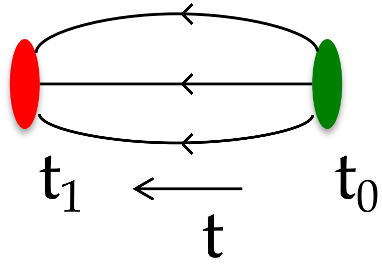
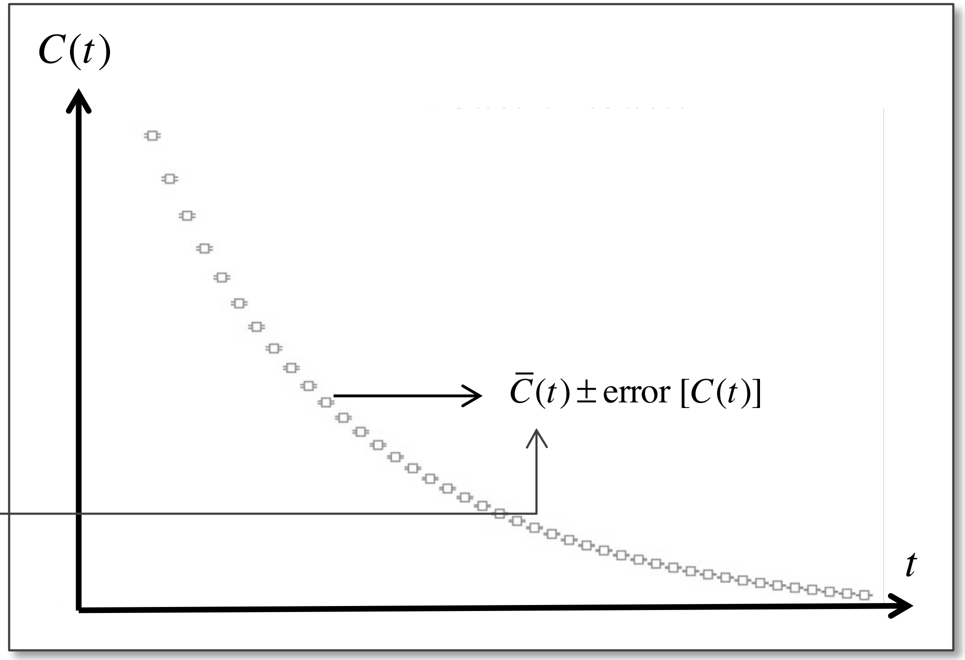


average over N gauge-field configurations $\{U_{x\mu}\}^i$ with $i = 1, 2, \ldots N$



$$C(t) = \langle 0|\phi(t)\phi^\dagger(0)|0\rangle \longrightarrow \langle\phi|e^{-Ht}|\phi\rangle = \sum_n \langle\phi|e^{-Ht}|n\rangle\langle n|\phi\rangle = \sum |\langle\phi|n\rangle|^2 e^{-E_n t}$$

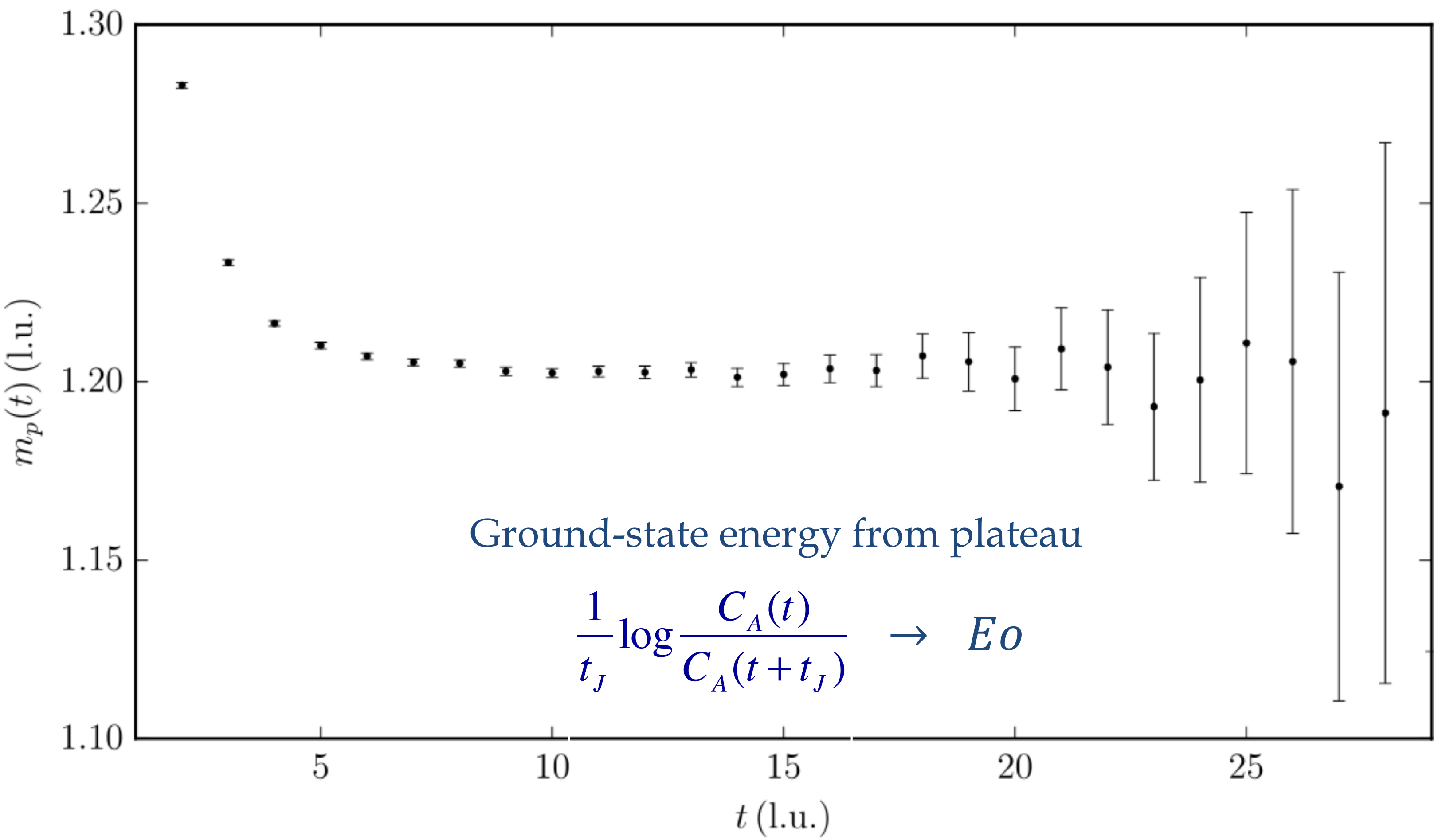
$$\phi(t) = e^{Ht}\phi\, e^{-Ht}$$

$$= Z_0^{snk} Z_0^{\dagger src} e^{-E^{(0)}t} + Z_1^{snk} Z_1^{\dagger src} e^{-E^{(1)}t} + \ldots$$

i.e. one can obtain the lowest energy state provided we see the large time exponential fall-off of the correlation function (Euclidean time evolution suppresses excited states)

LQCD DIRECT METHOD:
FV Energy levels from two-point correlation functions. Effective mass plot

$$p_\alpha(\mathbf{x},t) = \epsilon^{ijk} u^i_\alpha(\mathbf{x},t) \left(u^{j\mathsf{T}}(\mathbf{x},t) C\gamma_5 d^k(\mathbf{x},t) \right)$$



$$\frac{1}{t_J} \log \frac{C_A(t)}{C_A(t+t_J)} \rightarrow E_0$$

LQCD DIRECT METHOD:
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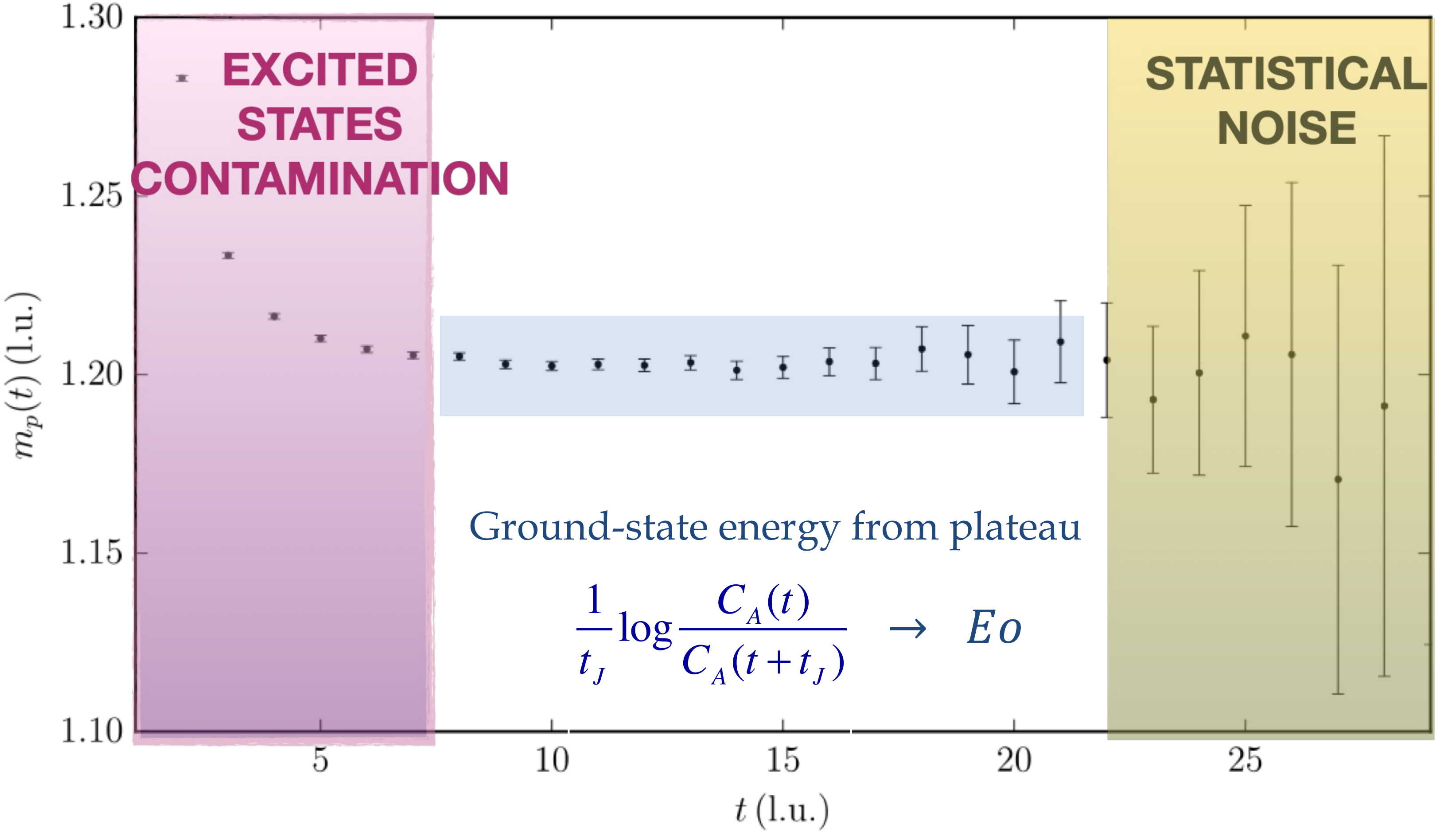


$$\frac{1}{t_J}\log\frac{C_A(t)}{C_A(t+t_J)} \rightarrow E_0$$

Signal-to-noise

Lepage, 1989

$$\text{signal} \sim \langle C \rangle \sim \langle 0|\mathcal{O}|0\rangle \quad \text{noise} \sim \sqrt{N\,\sigma^2} \sim \sqrt{N}\sqrt{\langle C^\dagger C\rangle - \langle C\rangle^2} \sim \sqrt{N}\sqrt{\langle 0|\mathcal{O}^\dagger\mathcal{O}|0\rangle - \langle 0|\mathcal{O}|0\rangle^2}$$

$$\frac{\text{signal}}{\text{noise}} \sim \frac{\langle 0|\mathcal{O}|0\rangle}{\sqrt{N}\sqrt{\langle 0|\mathcal{O}^\dagger\mathcal{O}|0\rangle - \langle 0|\mathcal{O}|0\rangle^2}}$$

Argument given by Lepage: for a system with N valence quarks lines (2 for mesons and 3 for baryons) the errors are controlled by the square of the correlator, which has 2N lines

Signal-to-noise

Lepage, 1989

$$\text{signal} \sim \langle C \rangle \sim \langle 0|\mathcal{O}|0\rangle \qquad \text{noise} \sim \sqrt{N\,\sigma^2} \sim \sqrt{N}\sqrt{\langle C^\dagger C\rangle - \langle C\rangle^2} \sim \sqrt{N}\sqrt{\langle 0|\mathcal{O}^\dagger\mathcal{O}|0\rangle - \langle 0|\mathcal{O}|0\rangle^2}$$

$$\frac{\text{signal}}{\text{noise}} \sim \frac{\langle 0|\mathcal{O}|0\rangle}{\sqrt{N}\sqrt{\langle 0|\mathcal{O}^\dagger\mathcal{O}|0\rangle - \langle 0|\mathcal{O}|0\rangle^2}}$$

pions

signal

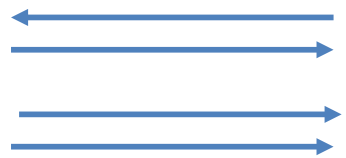
π

$\sim e^{-m_\pi t}$

noise

π

$\pi^\dagger$



$\sigma^2 \sim e^{-2m_\pi t}$

lowest energy state

Signal-to-noise

Lepage, 1989

signal $\sim \langle C \rangle \sim \langle 0|\mathcal{O}|0\rangle$ noise $\sim \sqrt{N\,\sigma^2} \sim \sqrt{N}\sqrt{\langle C^\dagger C\rangle - \langle C\rangle^2} \sim \sqrt{N}\sqrt{\langle 0|\mathcal{O}^\dagger\mathcal{O}|0\rangle - \langle 0|\mathcal{O}|0\rangle^2}$

$$\frac{\text{signal}}{\text{noise}} \sim \frac{\langle 0|\mathcal{O}|0\rangle}{\sqrt{N}\sqrt{\langle 0|\mathcal{O}^\dagger\mathcal{O}|0\rangle - \langle 0|\mathcal{O}|0\rangle^2}}$$

pions

$$\langle C(t)\rangle = \left\langle \left(\sum_x \pi^-(\vec{x},t)\right)\left(\pi^+(\vec{0},0)\right)\right\rangle \rightarrow A_0\, e^{-m_\pi t}$$

$$N\sigma^2 \sim \left\langle C^+(t)C(t)\right\rangle - \left\langle C(t)\right\rangle^2$$

$$= \left\langle \left(\sum_x \pi^-(\vec{x},t)\right)\left(\sum_y \pi^+(\vec{y},t)\right)\left(\pi^+(\vec{0},0)\right)\left(\pi^-(\vec{0},0)\right)\right\rangle - \left\langle \left(\sum_x \pi^-(\vec{x},t)\right)\left(\pi^+(\vec{0},0)\right)\right\rangle^2$$

$$\rightarrow \left(A_2 - A_0^2\right)e^{-2m_\pi t}$$

$$\frac{\sigma(t)}{\langle C(t)\rangle} \sim \frac{\sqrt{\left(A_2 - A_0^2\right)}\, e^{-m_\pi t}}{\sqrt{N}A_0\, e^{-m_\pi t}} \sim \frac{1}{\sqrt{N}}$$

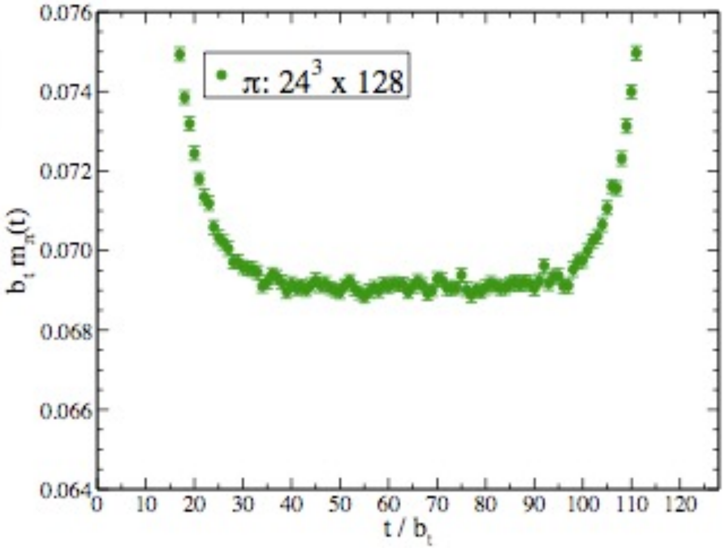
Signal-to-noise

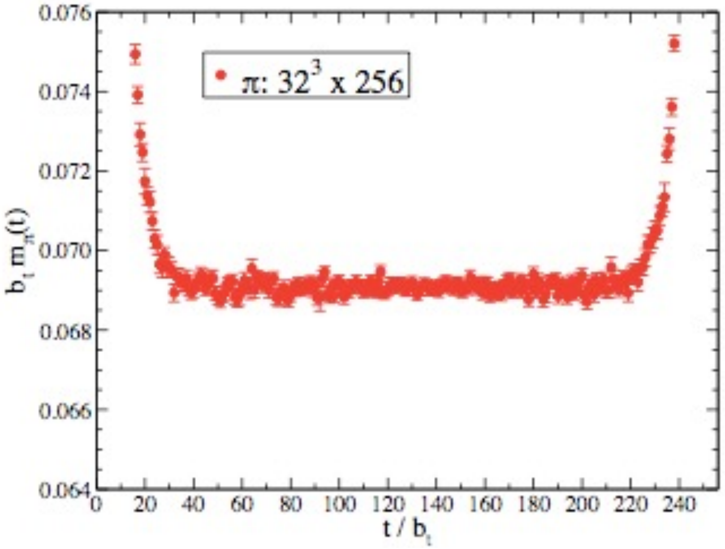
Lepage, 1989

$$\text{signal} \sim \langle C \rangle \sim \langle 0|\mathcal{O}|0\rangle \quad \text{noise} \sim \sqrt{N\,\sigma^2} \sim \sqrt{N}\sqrt{\langle C^\dagger C\rangle - \langle C\rangle^2} \sim \sqrt{N}\sqrt{\langle 0|\mathcal{O}^\dagger\mathcal{O}|0\rangle - \langle 0|\mathcal{O}|0\rangle^2}$$

$$\frac{\text{signal}}{\text{noise}} \sim \frac{\langle 0|\mathcal{O}|0\rangle}{\sqrt{N}\sqrt{\langle 0|\mathcal{O}^\dagger\mathcal{O}|0\rangle - \langle 0|\mathcal{O}|0\rangle^2}} \sim \frac{\sqrt{\left(A_2 - A_0^2\right)}\,e^{-m_\pi t}}{\sqrt{N}A_0\,e^{-m_\pi t}} \sim \frac{1}{\sqrt{N}}$$

pions





noise-to-signal independent of time

Signal-to-noise problem in baryon systems

Lepage, 1989

$$\text{signal} \sim \langle C \rangle \sim \langle 0|\mathcal{O}|0\rangle \qquad \text{noise} \sim \sqrt{N\,\sigma^2} \sim \sqrt{N}\sqrt{\langle C^\dagger C\rangle - \langle C\rangle^2} \sim \sqrt{N}\sqrt{\langle 0|\mathcal{O}^\dagger\mathcal{O}|0\rangle - \langle 0|\mathcal{O}|0\rangle^2}$$

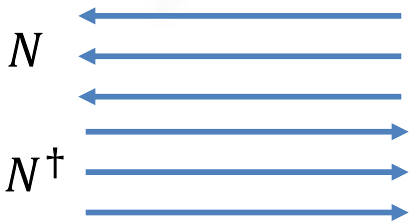
$$\frac{\text{signal}}{\text{noise}} \sim \frac{\langle 0|\mathcal{O}|0\rangle}{\sqrt{N}\sqrt{\langle 0|\mathcal{O}^\dagger\mathcal{O}|0\rangle - \langle 0|\mathcal{O}|0\rangle^2}}$$

nucleons

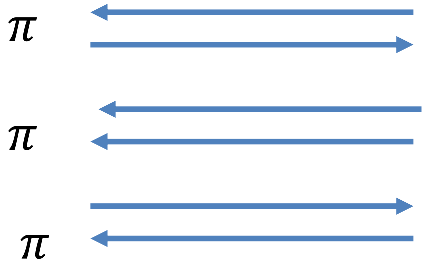
signal

$\sim e^{-m_p t}$

noise



$\sigma^2 \sim e^{-2mpt}$



$\sigma^2 \sim e^{-3m_\pi t}$

lowest energy state

Signal-to-noise problem in baryon systems

Lepage, 1989

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$$\frac{\text{signal}}{\text{noise}} \sim \frac{e^{-m_N t}}{\sqrt{N}\sqrt{e^{-3m_\pi t} - e^{-2m_N t}}} \quad \xrightarrow{t_{large}} \quad \frac{1}{\sqrt{N}} e^{-\left(m_N - \frac{3}{2}m_\pi\right)t}$$

the signal degrades with time

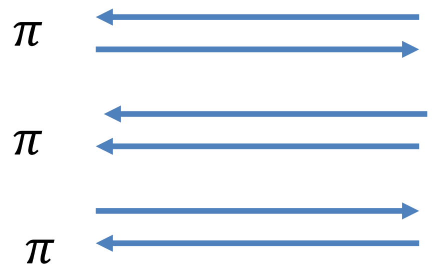
nucleons

signal

$\sim e^{-m_N t}$

noise

$\sigma^2 \sim e^{-2mNt}$



$\sigma^2 \sim e^{-3m_\pi t}$

lowest energy state

Signal-to-noise problem in baryon systems

Lepage, 1989

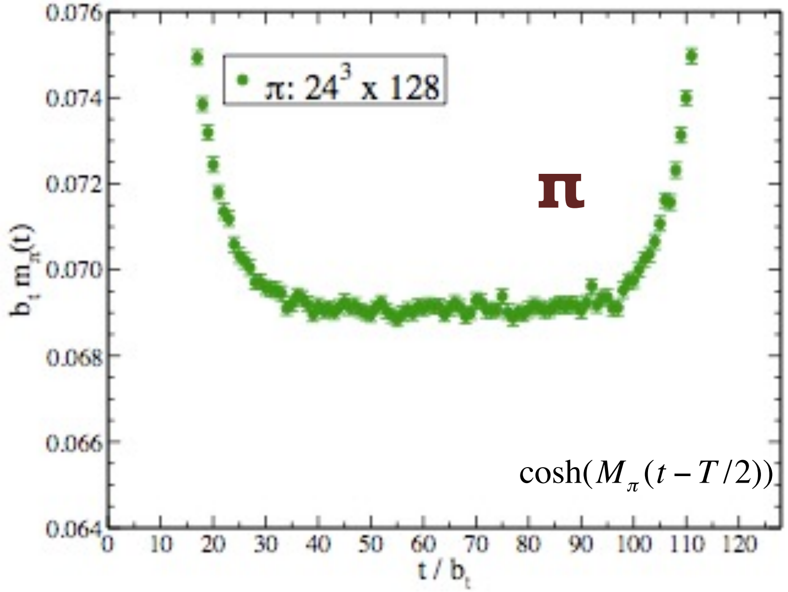
nucleons

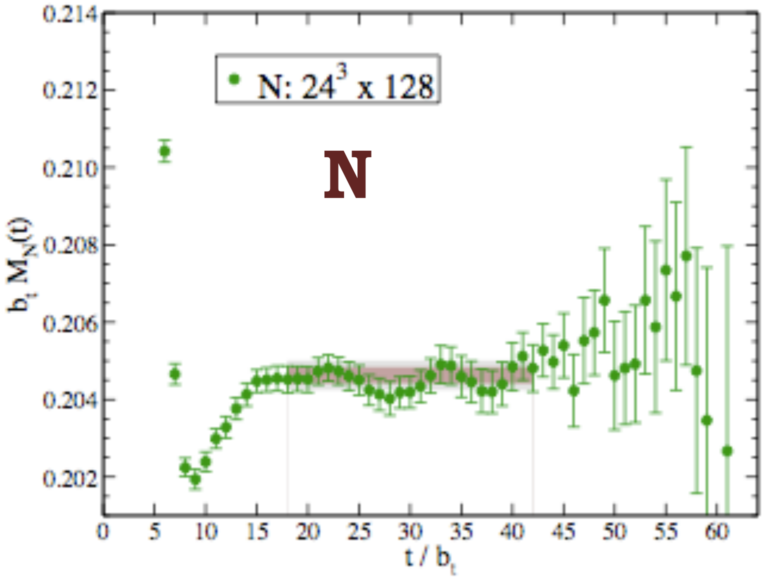
Important issue when working with baryons: NOISE!

$$\sigma^2(C) = \langle C C^\dagger \rangle - |\langle C \rangle|^2$$

exponential grow of noise

NPLQCD, arXiv:1104.4101 [hep-lat]





Tutorial this afternoon, with Sandra Tomás

Signal-to-noise problem in baryon systems

more severe degradation for A nucleons

Expectation is that for A nucleons:

$$\frac{\sigma}{\langle C \rangle} \sim \frac{\exp\left[A\left(M_N - \frac{3m_\pi}{2}\right)t\right]}{\sqrt{N}}$$

G. Parisi, Phys.Rept. 103 (1984)
G.P. Lepage, Boulder TASI (1989)
M.L. Wagman, M.J. Savage, Phys.Rev.D 96 (2017)

Signal-to-noise problem in baryon systems

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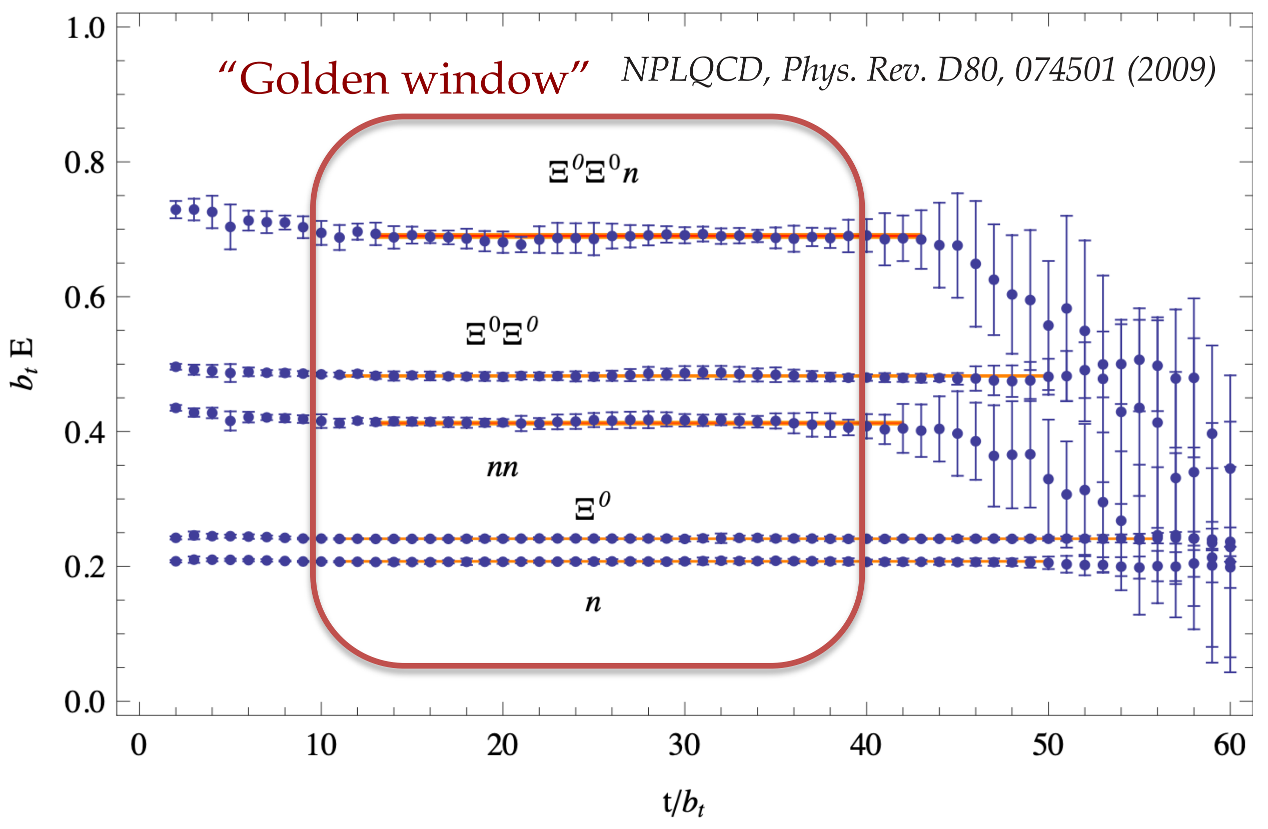
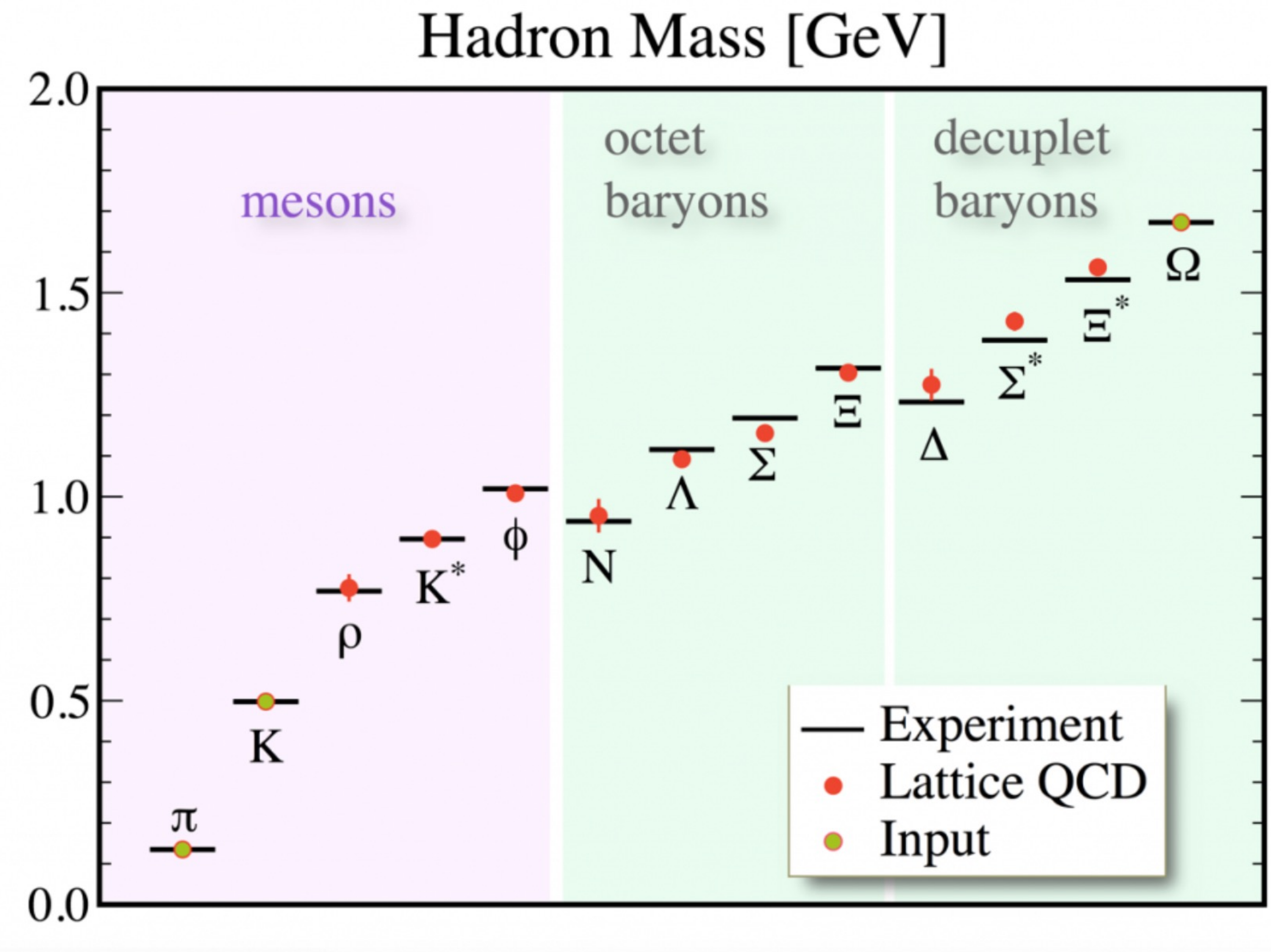


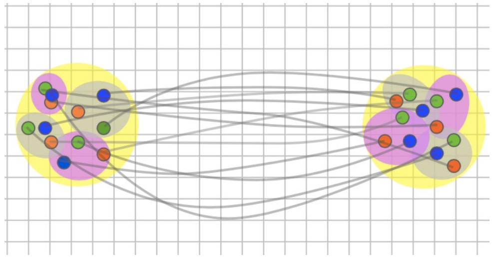
Successful examples: Light hadron spectrum



Phys. Rev. D 79 034504 (2008)

Successful examples: light nuclear systems

World @ 800 MeV



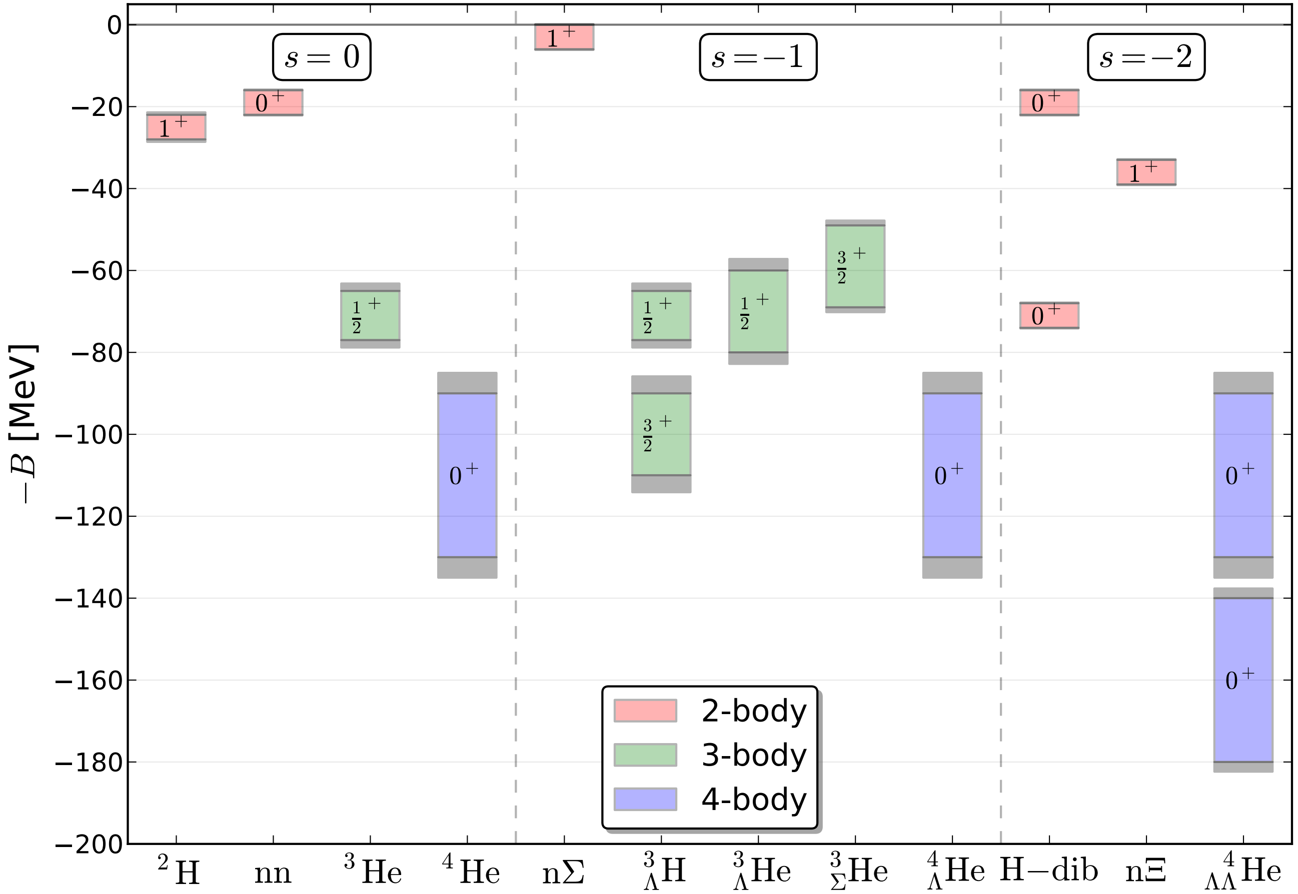
factorial growth in the number of contractions

NPLQCD Phys. Rev. D87 (2013) 3, 034506

$SU(3)_f$

NPLQCD

$m_\pi \sim 800$ MeV

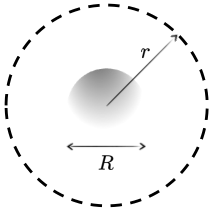


no e.m. interactions

(hadronic labels for (J^π, I, s, A) states)

M. Lüscher, Comm. Math. Phys. 105 (1986), Nuc. Phys. B 354 (1991)

Infinite
volume



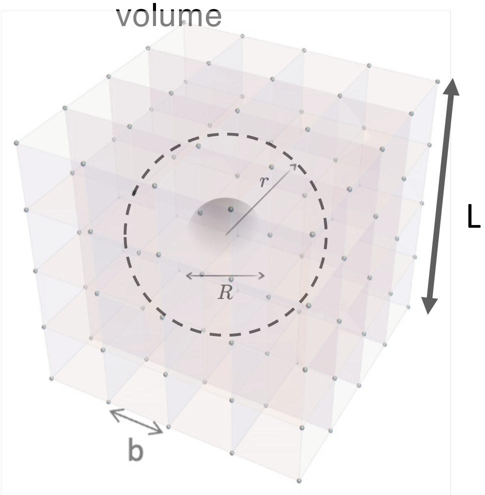
$$u_l(r;k) = \alpha_l(k) j_l(kr) + \beta_l(k) n_l(kr)$$

$$e^{2i\delta_l(k)} = \frac{\alpha_l(k) + i\beta_l(k)}{\alpha_l(k) - i\beta_l(k)}$$

10
2

M. Lüscher, Comm. Math. Phys. 105 (1986), Nuc. Phys. B 354 (1991)

finite
volume



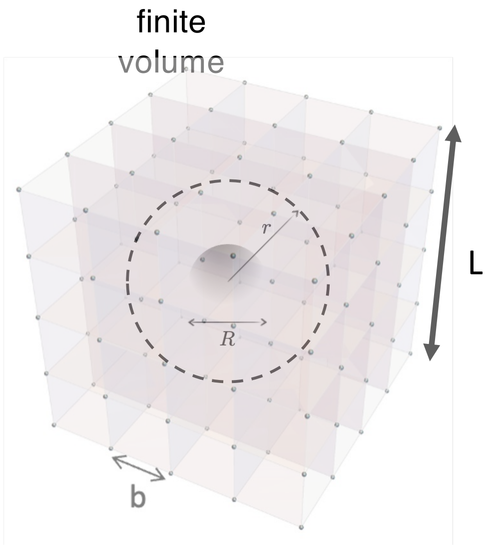
$$\det\left[(\mathcal{M}^{\infty})^{-1} + \delta\mathcal{G}^{V}\right] = 0$$

$(L \gg R)$

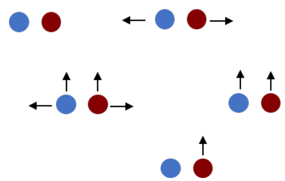
10
3

Scattering information in Euclidean space-time and FV

M. Lüscher, Comm. Math. Phys. 105 (1986), Nuc. Phys. B 354 (1991)



$(L \gg R)$



$$\det\left[(\mathcal{M}^{\infty})^{-1} + \delta\mathcal{G}^{V}\right] = 0$$

$\Delta E \rightarrow k*$

kinematic function

Generalized $\mathcal{Z}$ function

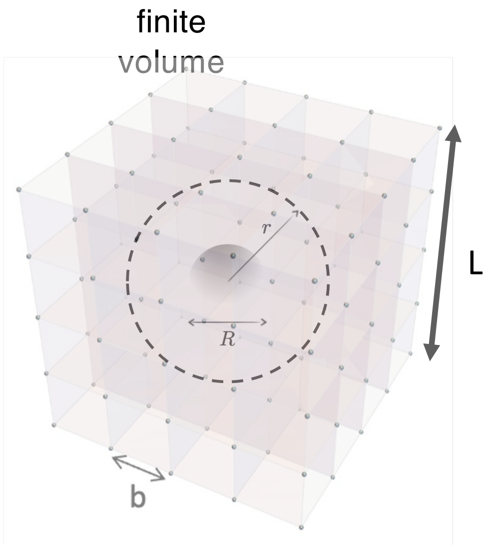
$$\mathcal{Z}^{\boldsymbol{d}}_{lm}(s;q^2) = \sum_{\boldsymbol{r}} \frac{r^l Y_{lm}(\hat{\boldsymbol{r}})}{\left(|\boldsymbol{r}|^2 - q^2\right)^s}$$

$$\boldsymbol{r} = \hat{\gamma}^{-1}\left(\boldsymbol{n} - \alpha\boldsymbol{d}\right), \ \boldsymbol{n} \in \mathbb{Z}^3$$

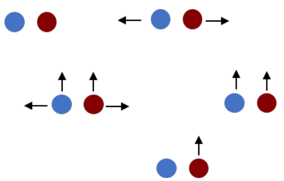
$$\alpha = \frac{1}{2}\left(1 + \frac{m_1^2 - m_2^2}{E^{*2}}\right)$$

10
4

M. Lüscher, Comm. Math. Phys. 105 (1986), Nuc. Phys. B 354 (1991)



$(L \gg R)$



$$\det\left[(\mathcal{M}^{\infty})^{-1} + \delta\mathcal{G}^{V}\right] = 0 \longrightarrow k^* \cot\delta = \frac{2}{\sqrt{\pi}L}\mathcal{Z}_{00}(1;(\tfrac{k^* L}{2\pi})^2)$$

$\Delta E \rightarrow k*$

kinematic function

Generalized $\mathcal{Z}$ function

$$\mathcal{Z}^{\boldsymbol{d}}_{lm}(s;q^2) = \sum_{\boldsymbol{r}} \frac{r^l Y_{lm}(\hat{\boldsymbol{r}})}{(|\boldsymbol{r}|^2 - q^2)^s}$$

$$\boldsymbol{r} = \hat{\gamma}^{-1}(\boldsymbol{n} - \alpha\boldsymbol{d}), \ \boldsymbol{n} \in \mathbb{Z}^3$$

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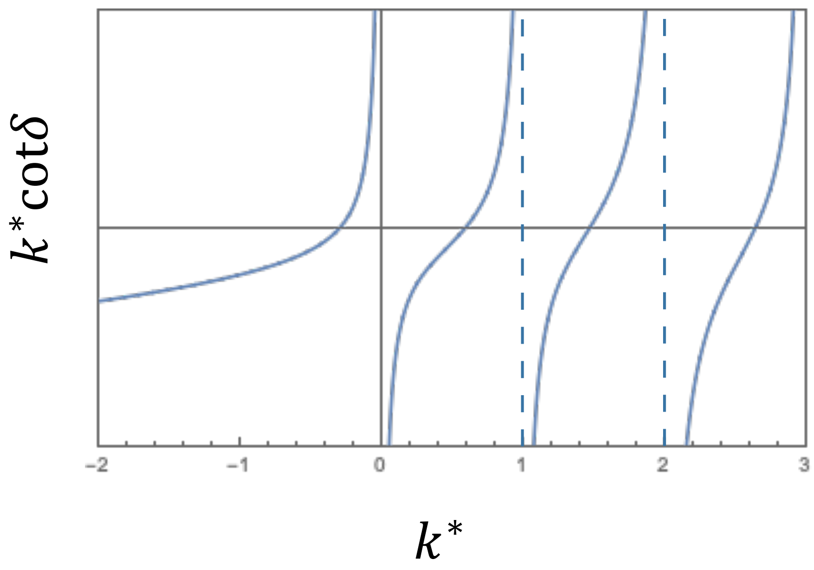
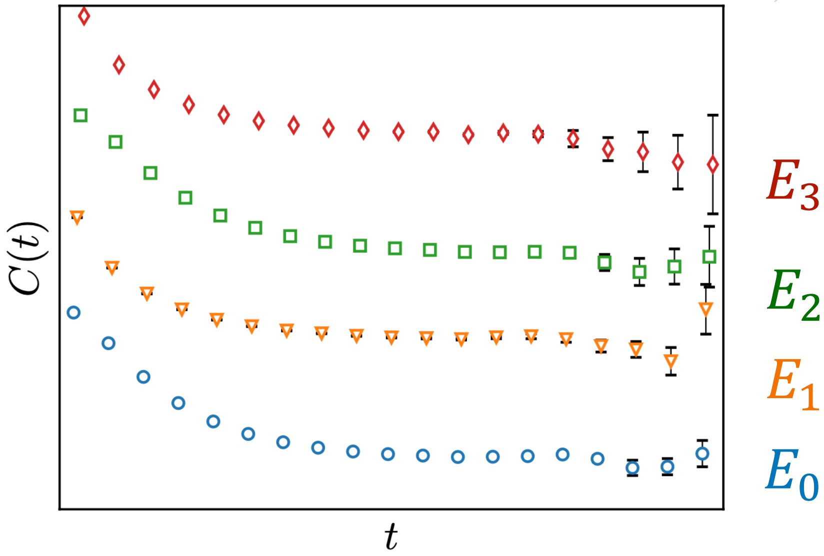
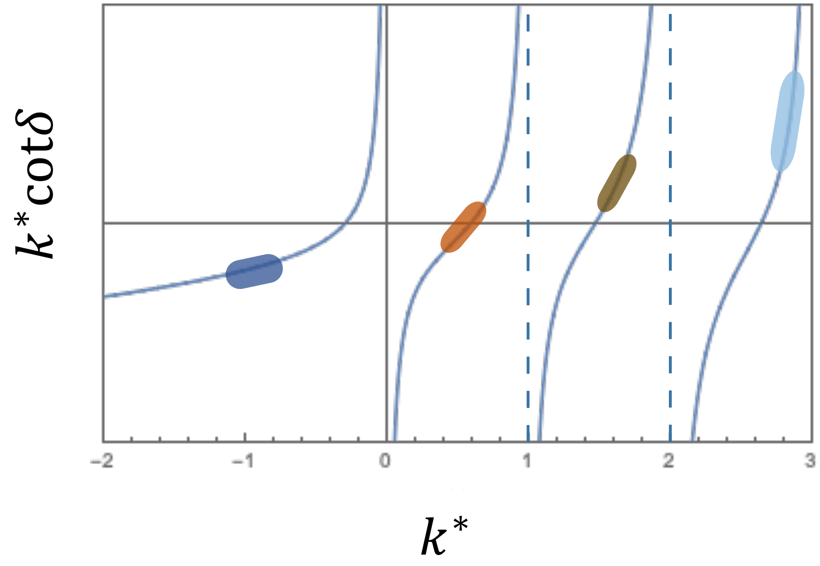


10
5

M. Lüscher, Comm. Math. Phys. 105 (1986), Nuc. Phys. B 354 (1991)

$$k^* \cot\delta = \frac{2}{\sqrt{\pi}L}\mathcal{Z}_{00}(1; (\tfrac{k^* L}{2\pi})^2)$$





$\Delta E \to k*$

10
8

$$k^* \cot\delta = \frac{2}{\sqrt{\pi}L}\mathcal{Z}_{00}(1; (\tfrac{k^* L}{2\pi})^2)$$

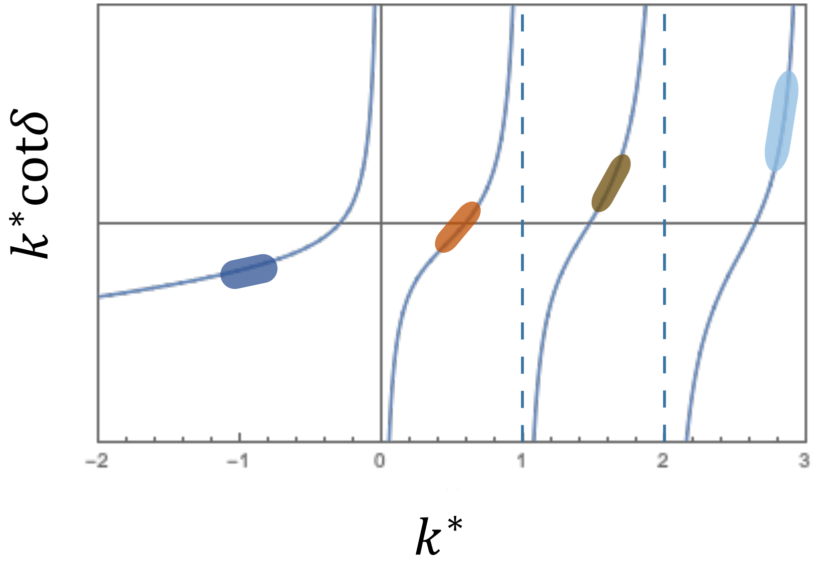
$k^{*2} < 0$

Beane, Bedaque, Parreño, Savage, PLB585 (2004)
Davoudi, Savage, PRD84 (2011)

$$|k^*| = \kappa^{(\infty)} + \frac{Z^2}{L}\left[6e^{-\kappa^{(\infty)}L} + \cdots\right]$$

B

$$k^* \cot\delta = \frac{2}{\sqrt{\pi}L}\mathcal{Z}_{00}(1; (\tfrac{k^* L}{2\pi})^2)$$



10
9

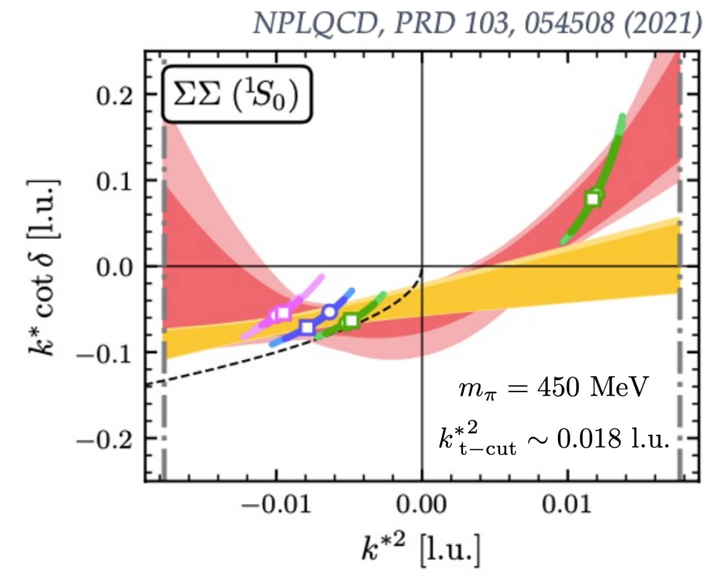
$$k^* \cot \delta = \frac{2}{\sqrt{\pi} L} \mathcal{Z}_{00}(1; (\frac{k^* L}{2\pi})^2)$$

$k^{*2} < 0$

Beane, Bedaque, Parreño, Savage, PLB585 (2004)
Davoudi, Savage, PRD84 (2011)

$$|k^*| = \kappa^{(\infty)} + \frac{Z^2}{L}\left[6e^{-\kappa^{(\infty)}L} + \cdots\right]$$

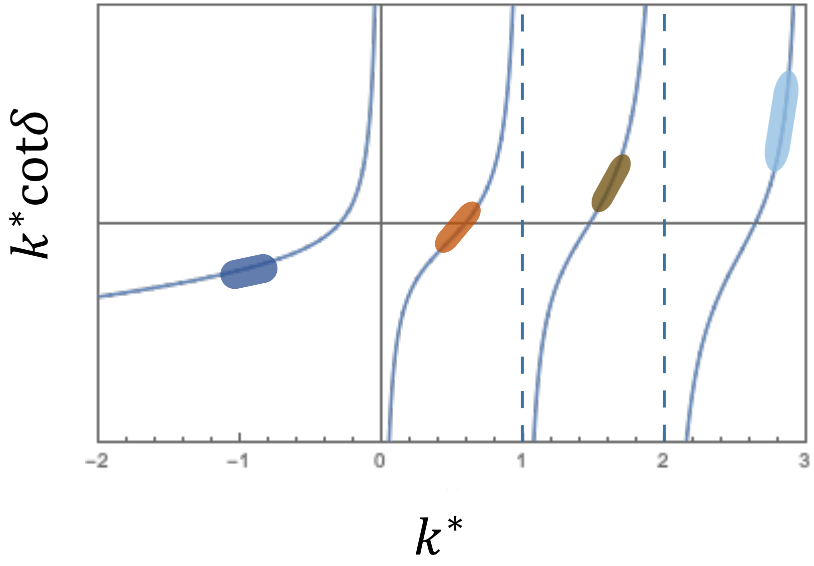
B



$$k^* \cot \delta = -\frac{1}{a} + \frac{1}{2} r k^{*2} + P k^{*4} + \mathcal{O}(k^{*6})$$

$\Delta E \rightarrow k*$

$$k^* \cot \delta = \frac{2}{\sqrt{\pi} L} \mathcal{Z}_{00}(1; (\frac{k^* L}{2\pi})^2)$$

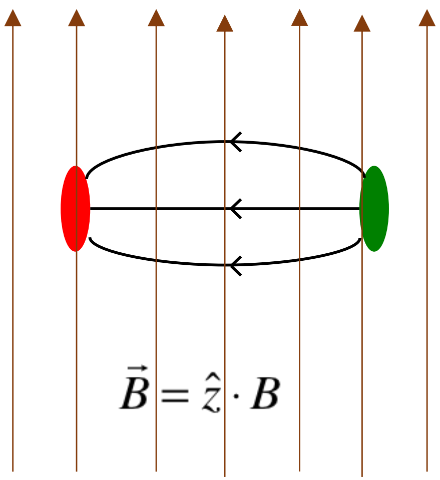


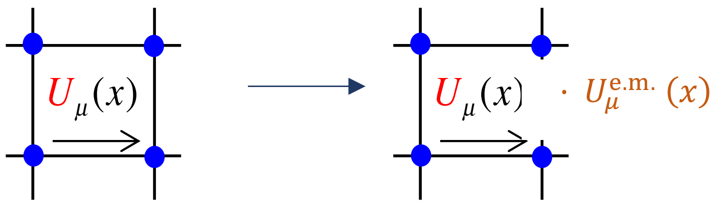
11
0

Other results (only if we have time)

One approach consists on taking a background field modifying the action

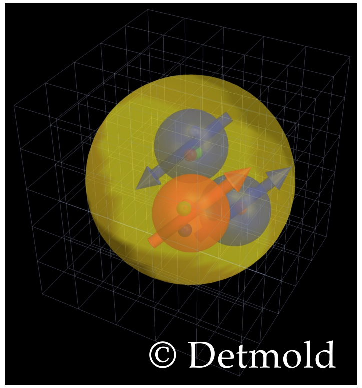
post-multiplication of the SU(3) color gauge links by fixed U(1) e.m. links





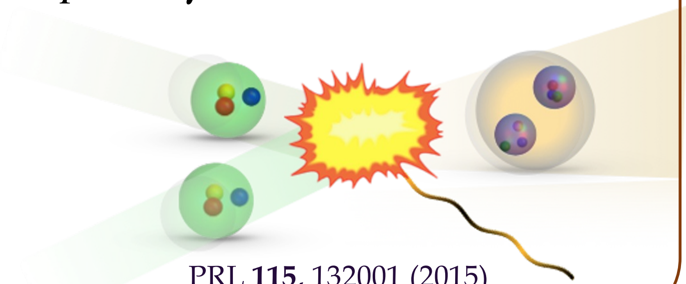
$$U_\mu^{\text{e.m.}}(x) = e^{iqA_\mu(x)} \in U(1)$$
$$= e^{-i\,qx_2B\delta_{\mu1}}\ e^{+i\,qx_1BN\delta_{\mu2}\delta_{x2.N-1}}$$

Magnetic Moments



PRD **95**, 114513 (2017)
PRL **116**, 112301 (2016)
PRD **92**, 114502 (2015)
PRL **113**, 252001 (2014)

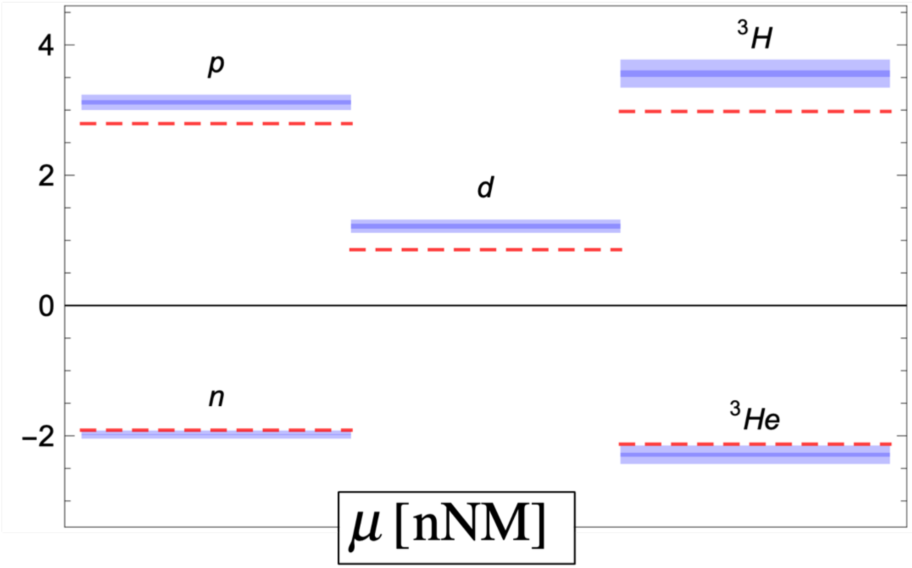
$np \to d\gamma$ cross section



PRL **115**, 132001 (2015)

Nuclear magnetic moments

NPLQCD, Phys. Rev .Lett. 113 (2014)



$$\text{nNM} = \frac{e}{2M_N^{\text{latt}}} = \frac{e}{2M_N(m_\pi^{\text{latt}})}$$

LQCD @ $m_\pi \sim 800$ MeV

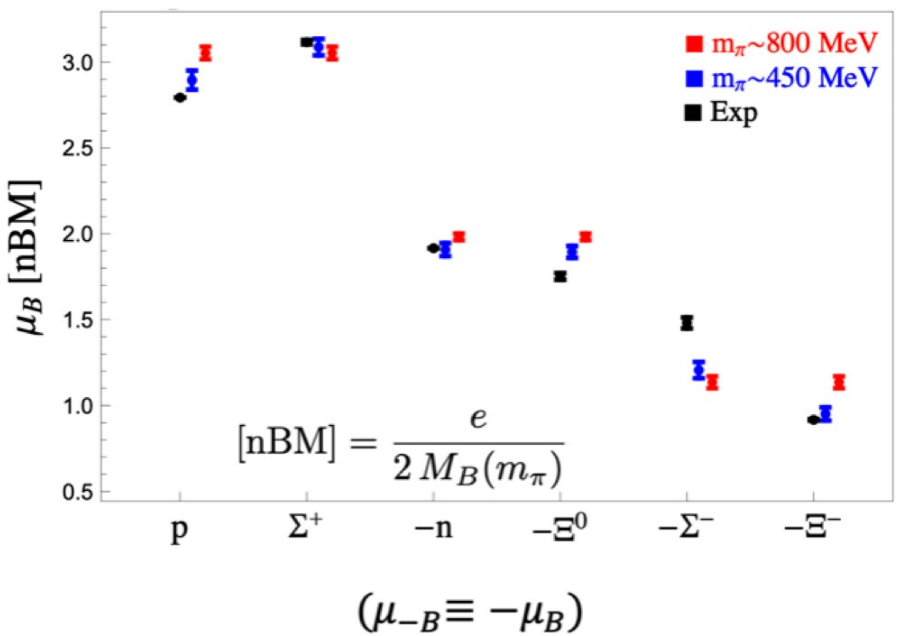
----------- experiment

Shell-model predictions

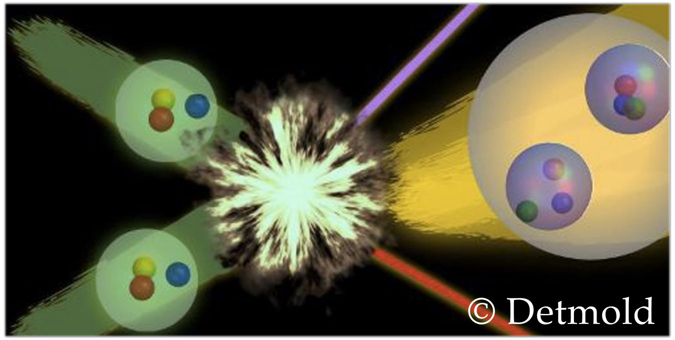
$$\mu(^3H) = \mu_p$$
$$\mu(^3He) = \mu_n$$
$$\mu_d = \mu_n + \mu_p$$

Octet baryon magnetic moments

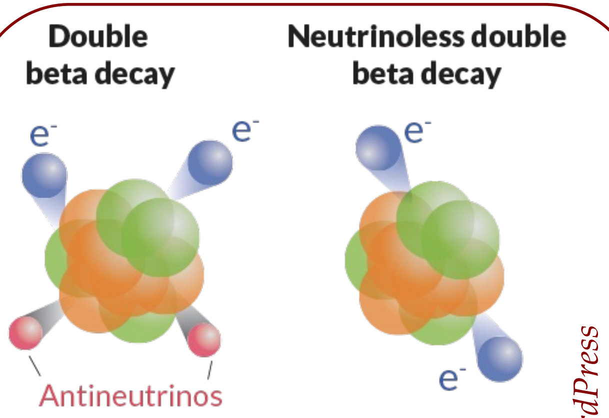
NPLQCD, PRD95, 114513 (2017)



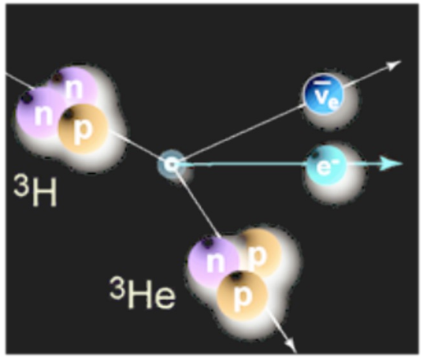
Another approach :
hadronic correlation functions are modified directly at the level of the valence quark propagators



Proton-Proton Fusion

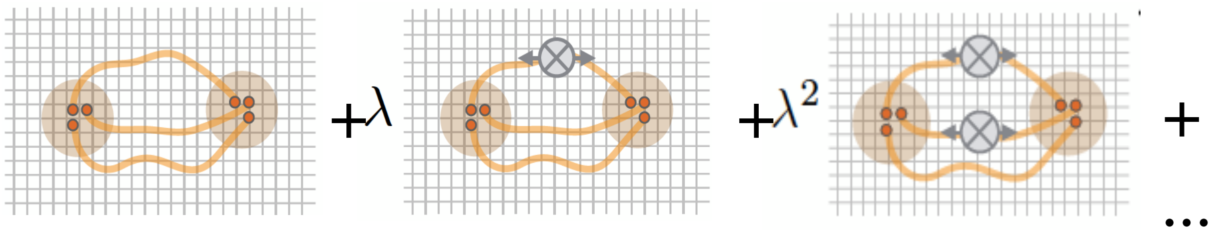


PRD 96, 054505 (2017)
PRL 119, 062003 (2017)



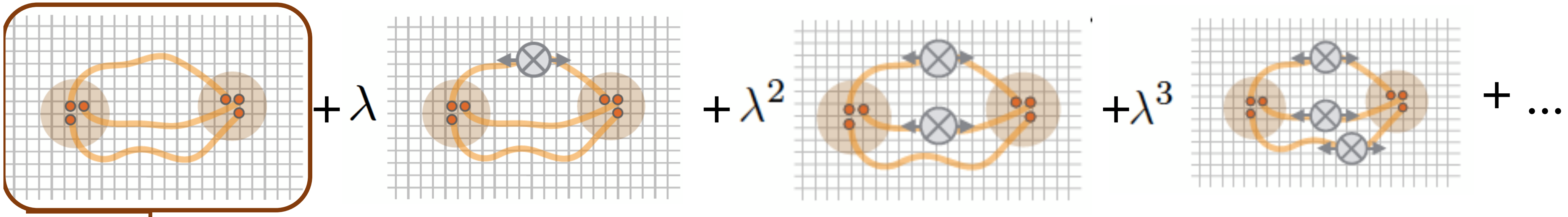
Tritium β Decay

PRL **119**, 062002 (2017)

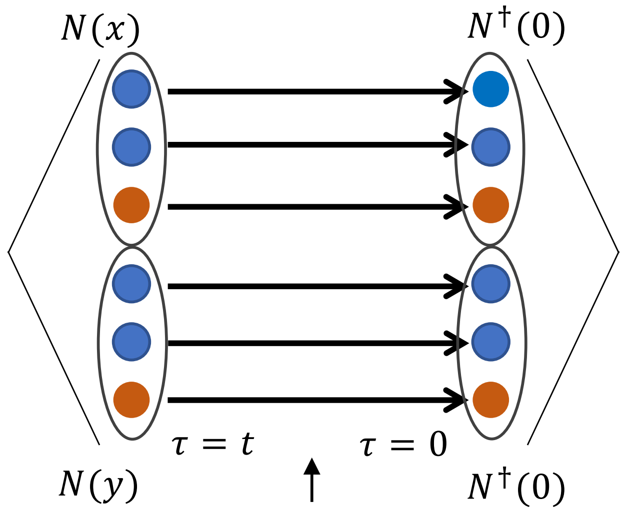


Savage et al. (NPLQCD) PRL 119, 062002 (2017); Bouchard et al (CALLATT), PRD96, 014504 (2017)

Interactions of nucleons/nuclei with external currents:



$$\sum_{\vec{p}_1+\vec{p}_2=\vec{P}} \; \sum_{\vec{x},\vec{y}} e^{\mathrm{i}\vec{p}_1\vec{x}+\mathrm{i}\vec{p}_2\vec{y}}$$



$$\sum_n |n\rangle \langle n|$$

$$\phi(t) = e^{Ht}\,\phi\; e^{-Ht}$$

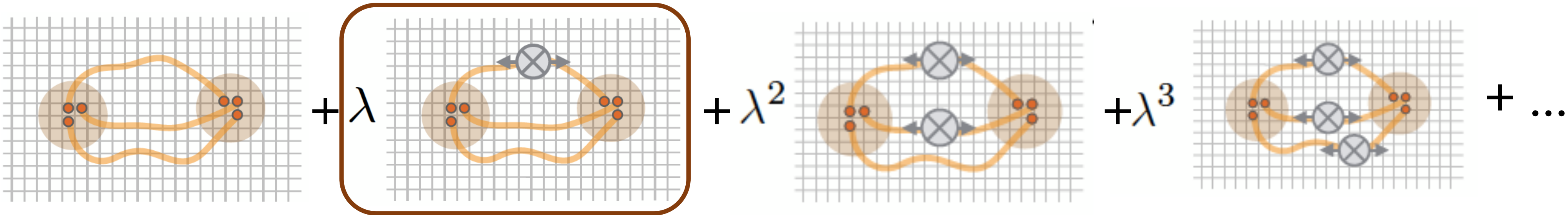
$$C_{\hat{O},\hat{O}'}\left(t,\vec{d},\Gamma^{\nu}\right) = \sum_{\vec{x}} e^{2\pi i \vec{d}\vec{x}/L}\;\Gamma^{\nu}\;\left\langle 0\middle|\hat{O}'(\vec{x},t)\,\hat{O}^{\dagger}(\vec{0},0)\middle|0\right\rangle$$

projected into total momentum $\frac{2\pi\vec{d}}{L}$

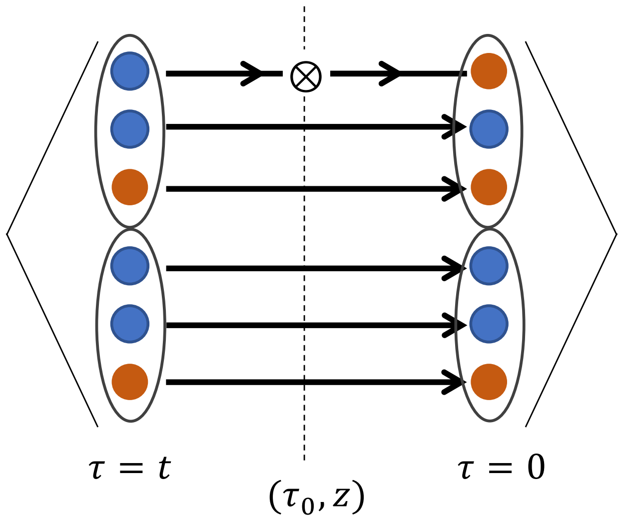
$$= \underbrace{Z_0^{snk}\, Z_0^{\dagger\, src}\; e^{-E^{(0)}t}}_{\text{dominates at large t}} + Z_1^{snk}\, Z_1^{\dagger\, src}\; e^{-E^{(1)}t} + \cdots$$

One obtains the energy spectrum fom the time dependence of ***correlation functions***

Interactions of nucleons/nuclei with external currents:

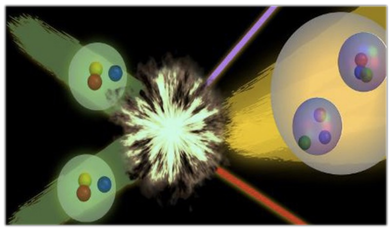


$$\lambda \sum_{\tau_0=0}^{t} \sum_{z}$$

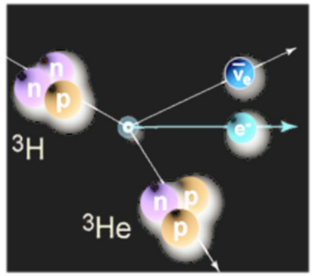


(sum over all possible insertions on quark lines)

linear response gives axial matrix element

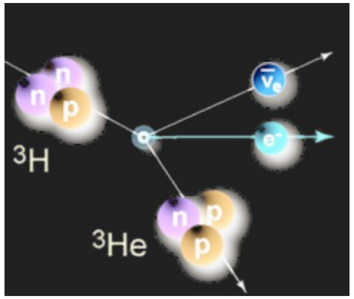


$pp \rightarrow d\, e^+ \nu_e$

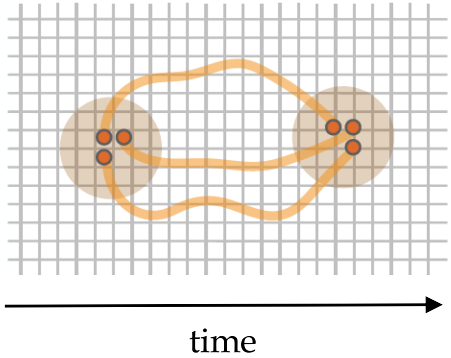


Gamow-Teller m.e

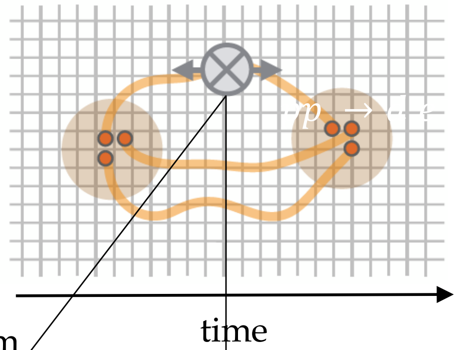
nuclear matrix elements ⟷ linear response in the compound correlator



Gamow-Teller m.e.
(axial current)



+ λ



+ ...

courtesy of P. Shanahan

implicit sum

$$C^{(h\sigma)}_{\lambda_q}(t) = \Gamma_{\beta\alpha}\sum_{\boldsymbol{x}}\left(\langle 0|\chi^h_\alpha(\boldsymbol{x},t)\overline{\chi}^h_\beta(0)|0\rangle + \lambda_q\sum_{\boldsymbol{y}}\sum_{\tau=0}^{t}\langle 0|\chi^h_\alpha(\boldsymbol{x},t)O^{(q)}(\boldsymbol{y},\tau)\overline{\chi}^h_\beta(0)|0\rangle\right) + \mathcal{O}(\lambda_q^2)$$

parity and spin projection

h={p, n, d, nn, np ($^1S_0$),pp,^{3}H, ^{3}He}

constant background field strength parameter

$$O^{(q)} = \overline{q}\Upsilon q$$

$$\Upsilon = \{1, \gamma_\mu\gamma_5, i\sigma_{\mu\nu}\}$$

scalar, axial, tensor

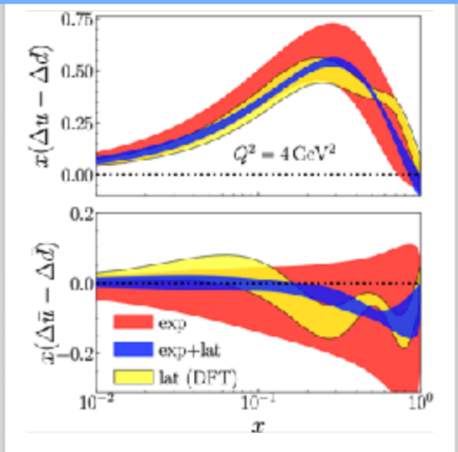
(polynomial of maximum order $\lambda_u^{Nu}\ \lambda_d^{Nd}$)

Other results in the hadronic sector I will not cover

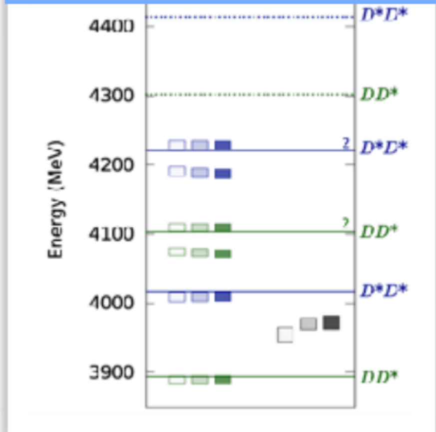
Modern day lattice QCD calculations

ISMD21: **[M. Constantinou, Tuesday, 16.35CET]**

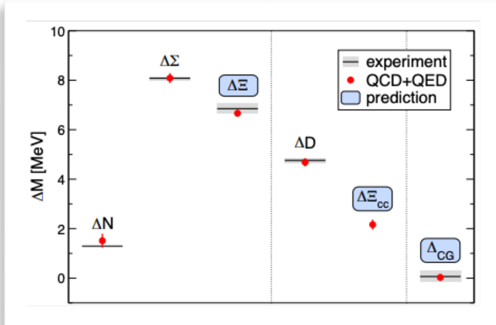
ISMD21: **[J. Dudek, Thursday, 16.35CET]**



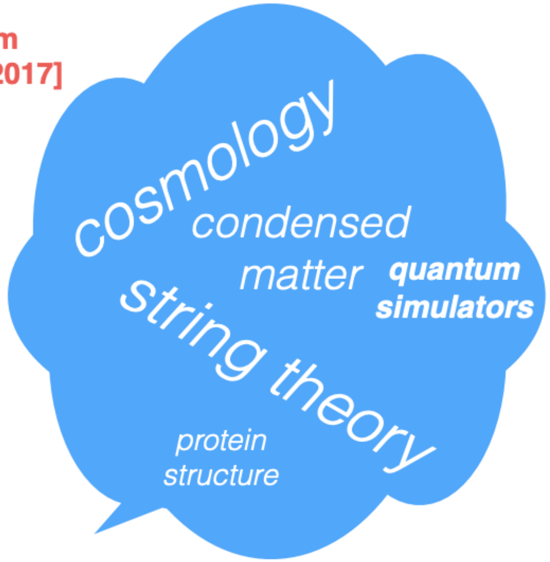
Lattice PDFs [Bringewatt, Sato, Melnitchouk, Qiu, Steffens, Constantinou, 2020]

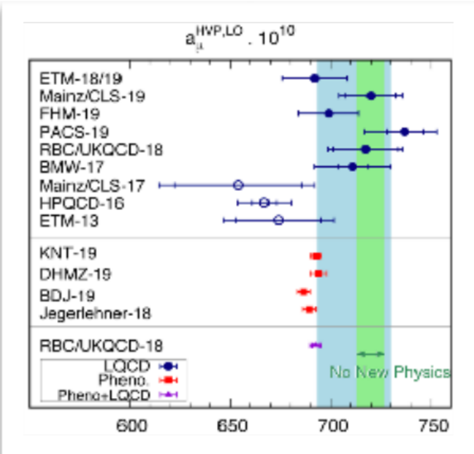


Double-charm FV energy spectrum [Cheung, Thomas, Dudek, Edwards 2017]

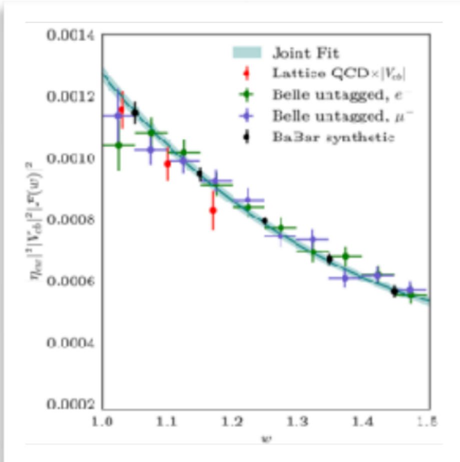


M_p-M_n [Borsanyi et. al 2014]





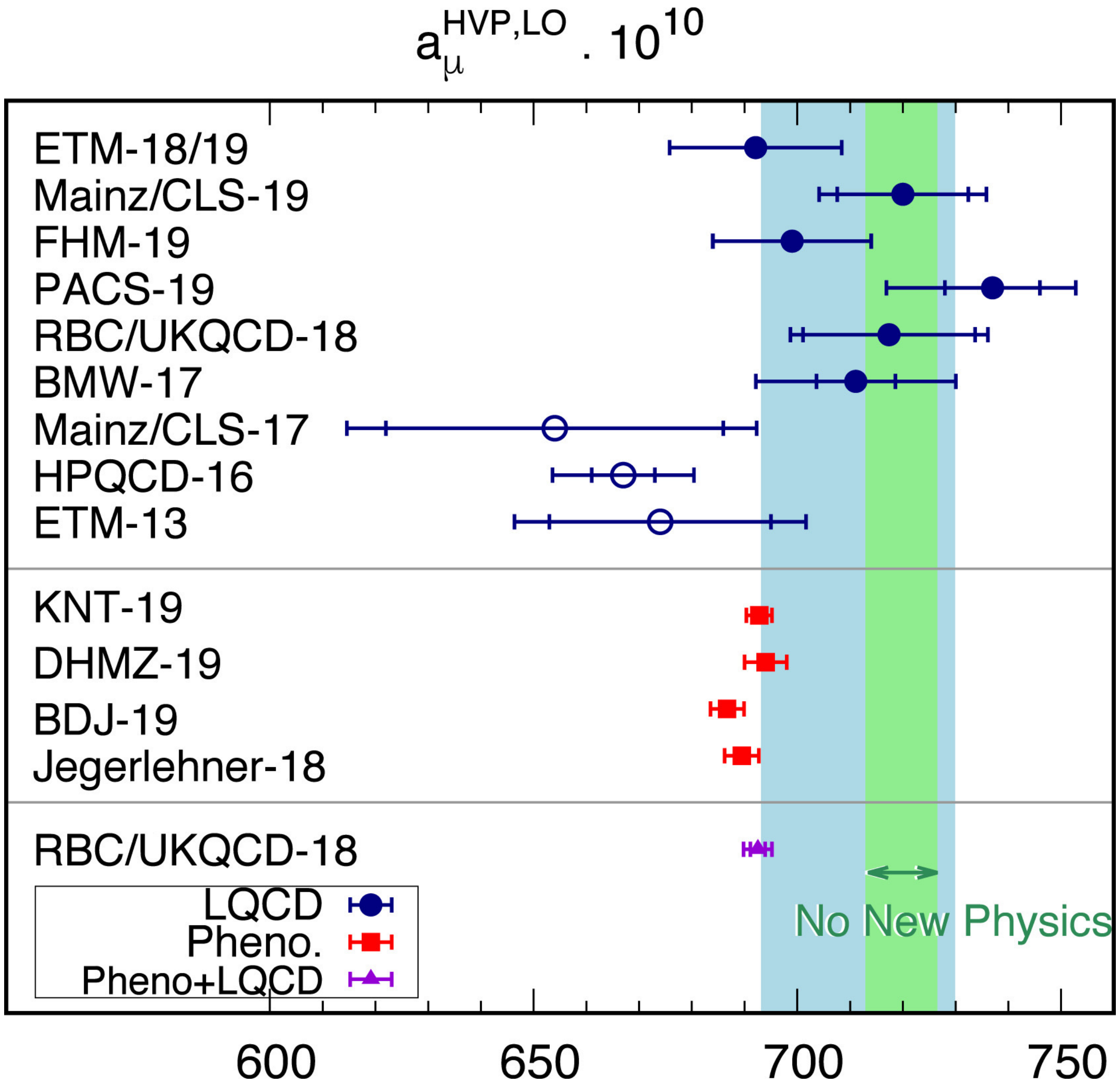
muon g-2: HVP [White paper, Muon g-2 Theory Initiative, Aoyama et al. 2020]



$|V_{cb}|$ from $B \to D^* l\nu$ [Bazavov et al. 2021, arxiv:2105.14019]

The anomalous magnetic moment of the muon in the Standard Model

T. Aoyama, et al, Phys. Rept. 887 (2020) 1–166



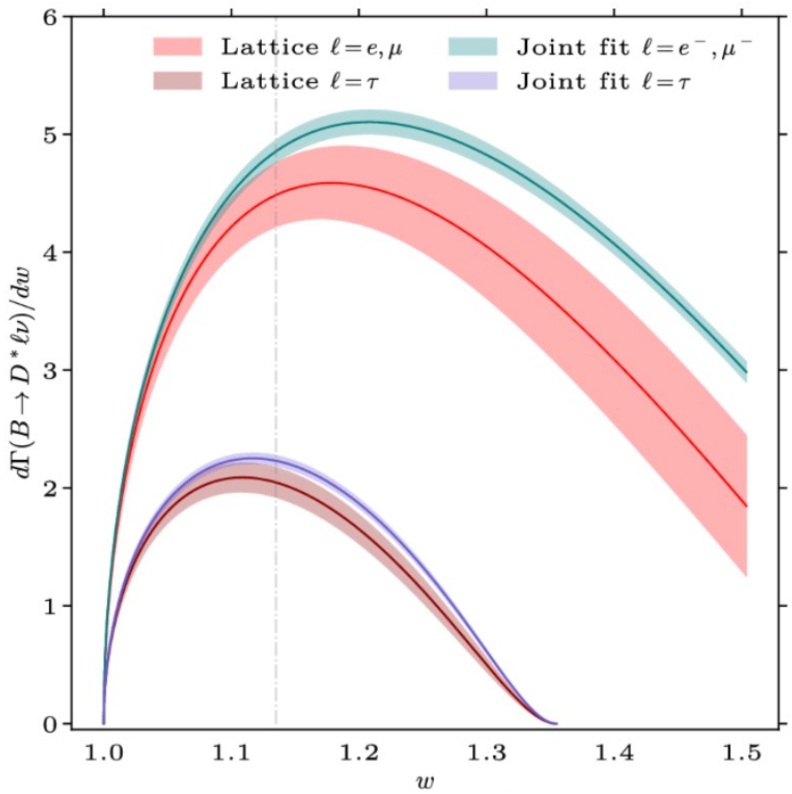
New Physics searches in the heavy flavour sector

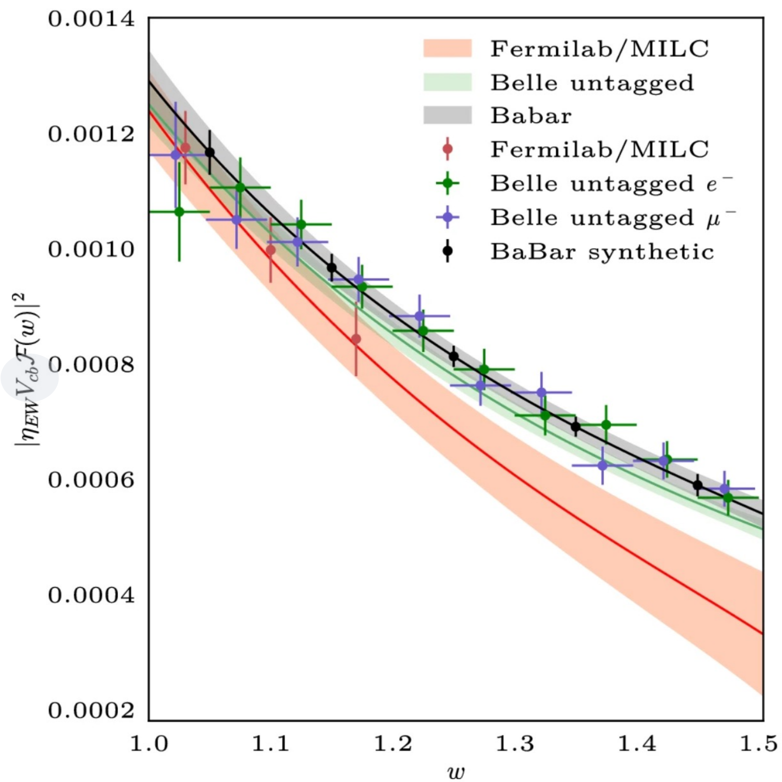
Searches for rare processes and for tiny deviations from Standard model expectations

For ex., lepton-flavor-universality-violating observables in B-meson semileptonic decays

$$R(D^{(*)}) \equiv \frac{\mathcal{B}(B \to D^{(*)}\tau\nu_\tau)}{\mathcal{B}(B \to D^{(*)}\ell\nu_\ell)}, \qquad \ell = e, \mu$$

$$V_{\rm CKM} = \begin{pmatrix} V_{\rm ud} & V_{\rm us} & V_{\rm ub} \\ V_{\rm cd} & V_{\rm cs} & V_{\rm cb} \\ V_{\rm td} & V_{\rm ts} & V_{\rm tb} \end{pmatrix}$$





A. Bazarov, et al., Eur. Phys. J. C (2022) 82:1141; https://doi.org/10.1140/epjc/s10052-022-10984-9

Lattice quantum chromodynamics. Practical Essentials.
F. Knechtli, M. Günther, M. Peardon
Springer, DOI 10.1007/978-94-024-0999-4

Quantum Chromodynamics on the Lattice. An introductory presentation
C. Gattringer, C.B. Lang
Lect. Notes Phys. 788 (Springer, Berlin Heidelberg 2010),
DOI 10.1007/978-3-642-01850-3

https://github.com/LatticeQCD

TAE – Lattice tutorial

Assumpta Parreño and Sandra Tomás, Universitat de Barcelona

- Correlation function for the pion, nucleon and two nucleons, using real lattice data (generated by the NPLQCD collaboration)

- Processing with Jackknife and bootstrap methods

- Fitting the Effective mass plots: constant, exponentials

- Analyzing the noise (signal-to-noise)

https://github.com/assumpg/TAE-School-LQCD