QCD+QED simulations

With C* boundary conditions

International Meetings on Fundamental Physics and XV CPAN days

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RC* collaboration

- IFCA (Santander):
  Dr. Isabel Campos, Dr. Gaurav Ray, Sara Rosso
- Humboldt University (Berlin):
  Prof Dr. Agostino Patella, Alessandro Cotellucci, Jens Lücke
- ETH (Zurich):
  Anian Altherr, Dr. Marco Catillo, Roman Gruber, Dr. Tim Harris,
  Prof. Dr. Marina Krstić Marinković, Dr. Letizia Parato, Paola Tavella
- Università di Roma Tor Vergata:
  Alessandro De Santis, Prof. Dr. Nazario Tantalo
- Trinity College (Dublin):
  Dr. Patrick Fritzsch
- IFIC (València):
  David Albandea

Summary of the talk

- **QCD+QED simulations**: why and how?
- Some remainders on **lattice QCD**
- **C* boundary conditions**
- **Results**: Lucius Bushnaq et al. First results on QCD+QED with C* boundary conditions. In: Journal of High Energy Physics 2022
    - Ensembles
    - Tuning
    - Lines of constant physics and hadron masses
- **Future objectives**

QCD+QED simulations in brief: why?

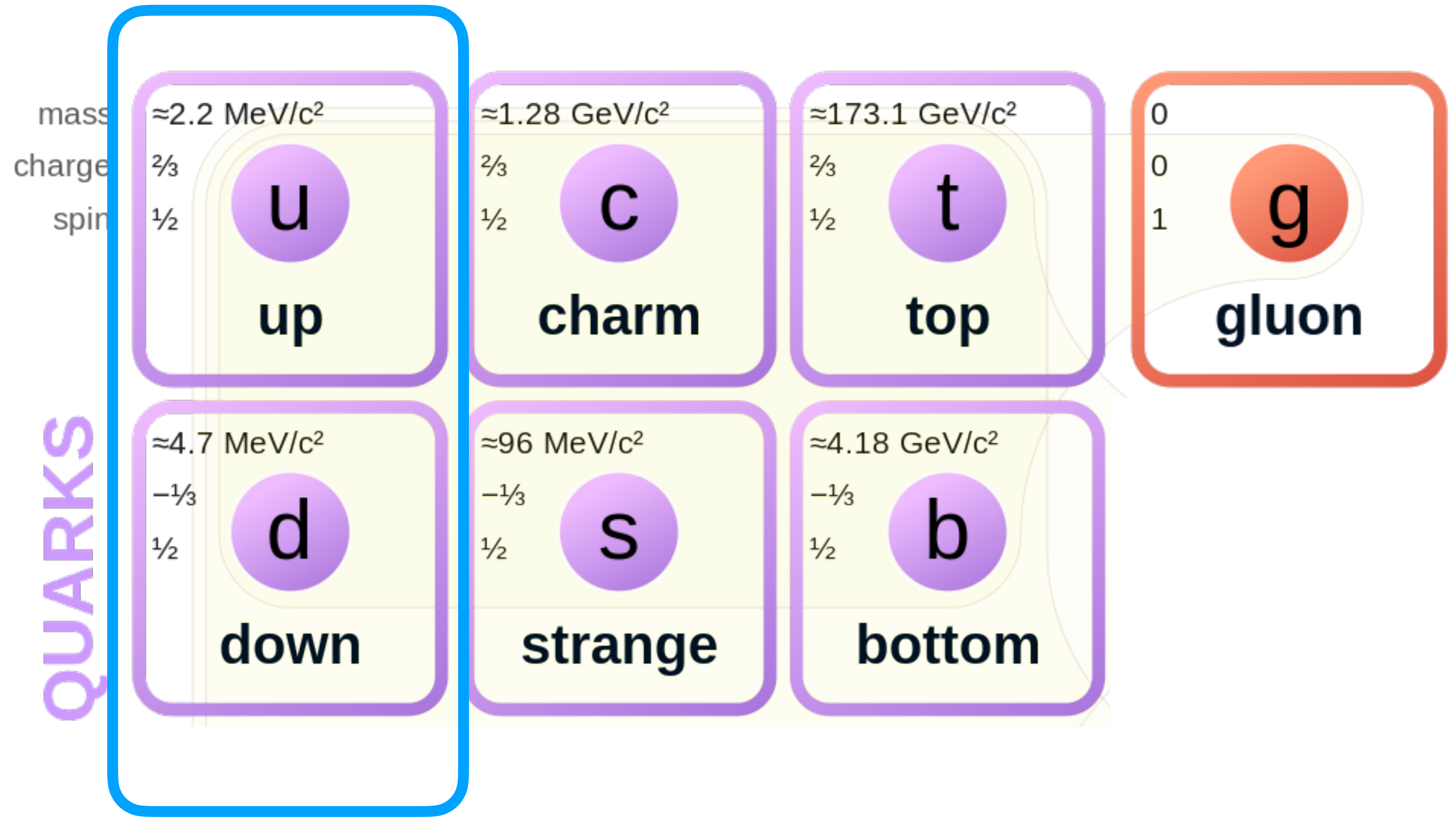
In order to achieve a percent or sub-percent level of precision in many hadronic measurements (such as meson masses and leading hadronic corrections to the muon $g-2$) **isospin breaking effects** have to be taken into account. They come from two sources:

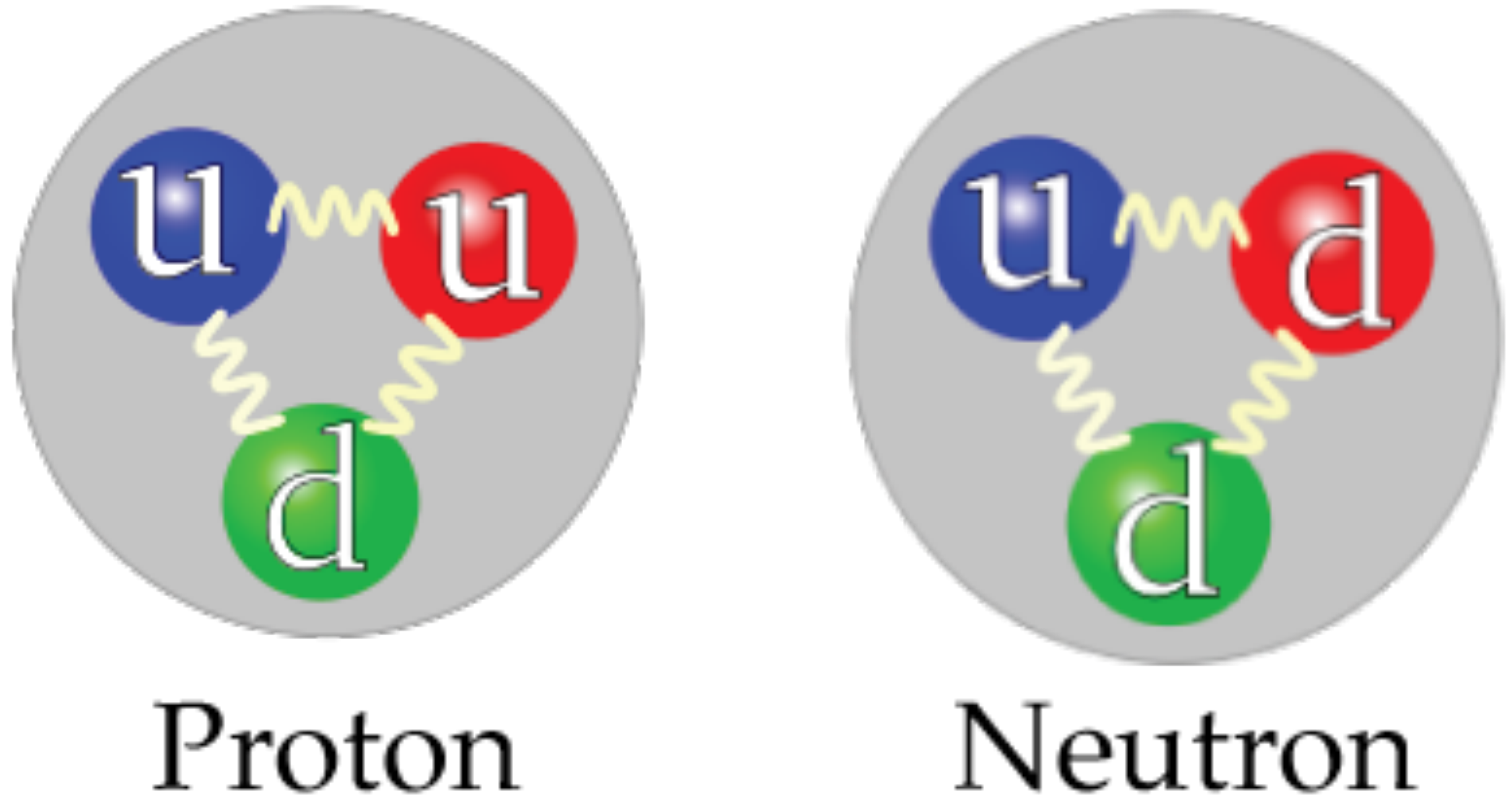
1. **Strong isospin breaking effects:** difference in the mass of the up and down quarks

2. **Electromagnetic isospin breaking effects:** difference in the electric charge of the up and down quarks

QCD+QED simulations in brief: why?

An example is the proton-neutron mass difference: $0.14\,\%$ of the average of the two masses, due to a combined effect of the two sources of isospin breaking.





QCD+QED in brief: how?

Lattice simulations have to be performed at finite volume, but in QED at finite volume with periodic boundary conditions in space, due to Gauss law, charged states are impossible:

$$Q = \int_0^L dx^3 \rho(x) = \int_0^L dx^3 \nabla \cdot E(x) = 0$$

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C* boundary conditions

A solution explored by our collaboration is the introduction of C* boundary conditions in space: charge conjugation of the fermionic and gauge fields at the boundary.

In this way the $U(1)$ gauge field is antiperiodic and :

$$Q = \int_0^L dx^3 \rho(x) = \int_0^L dx^3 \nabla \cdot E(x) \neq 0$$

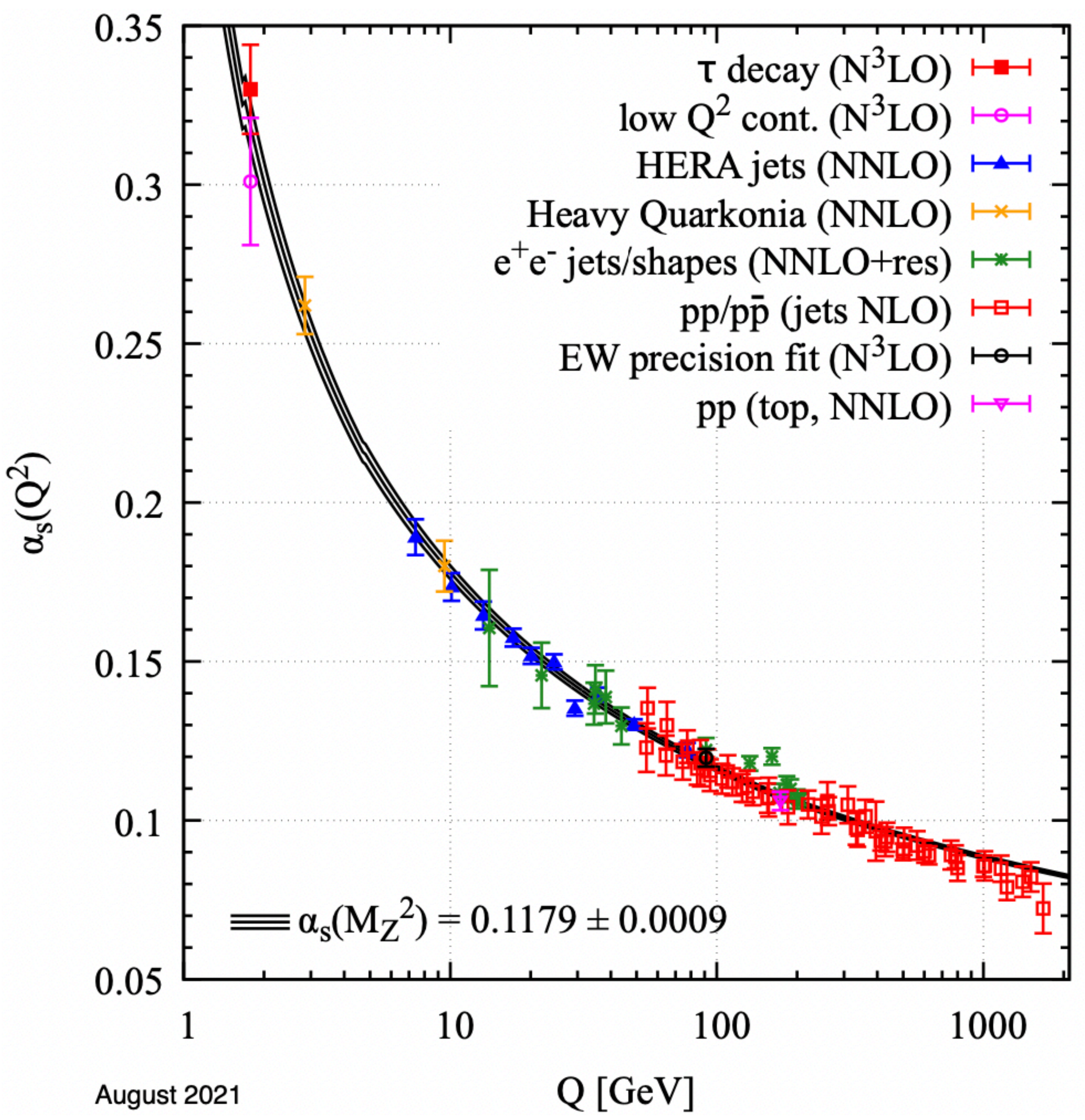
This approach preserves locality, translational invariance and gauge invariance at all stages of the calculation (as in the continuum theory).

Asymptotic freedom

A crucial property of QCD is asymptotic freedom: the theory becomes free in the high energy limit, while at low energy the theory is strongly coupled.

Perturbation theory is an expansion in a small coupling.

QCD is a non-perturbative theory at low energy, needs different techniques.

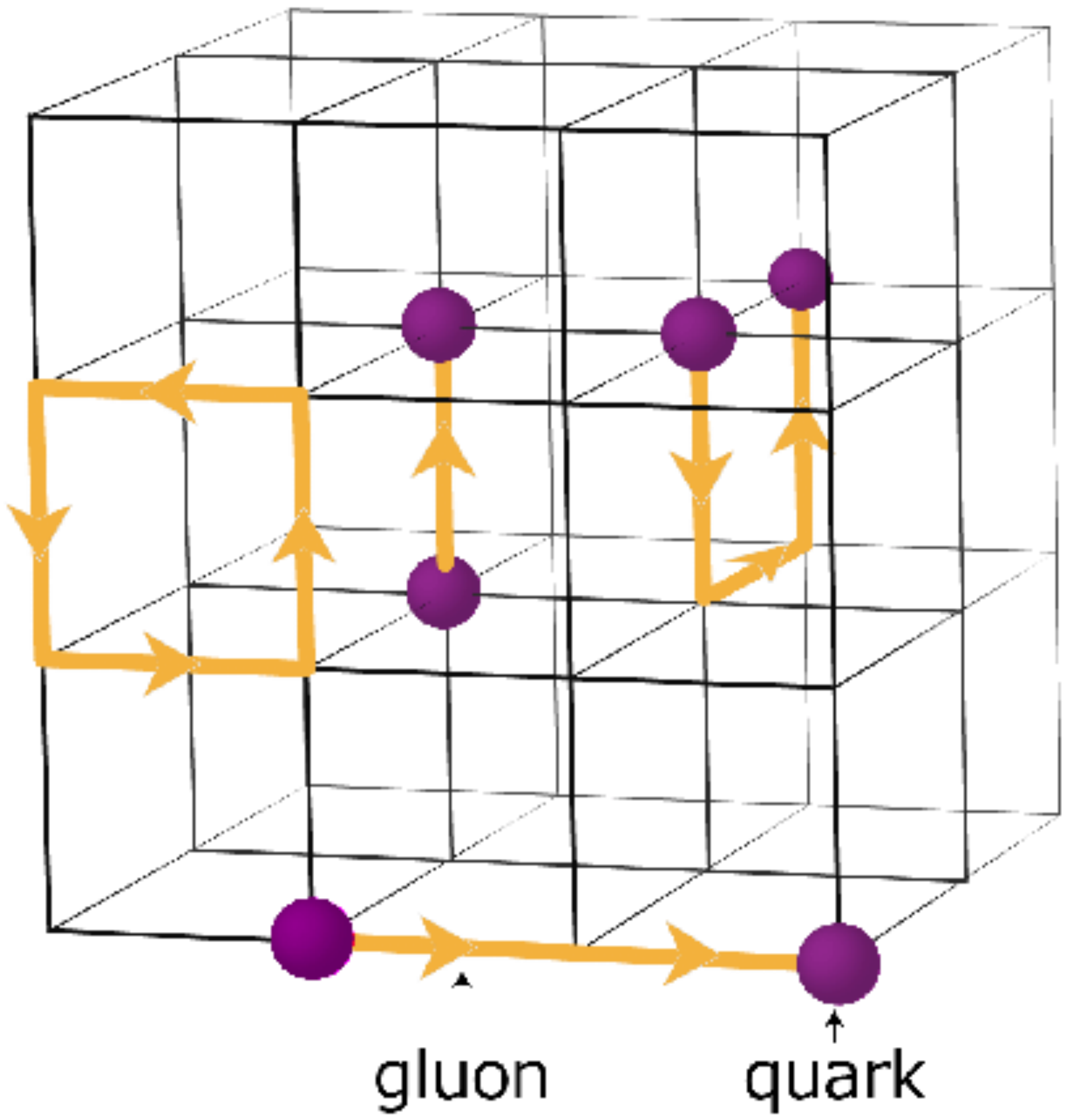


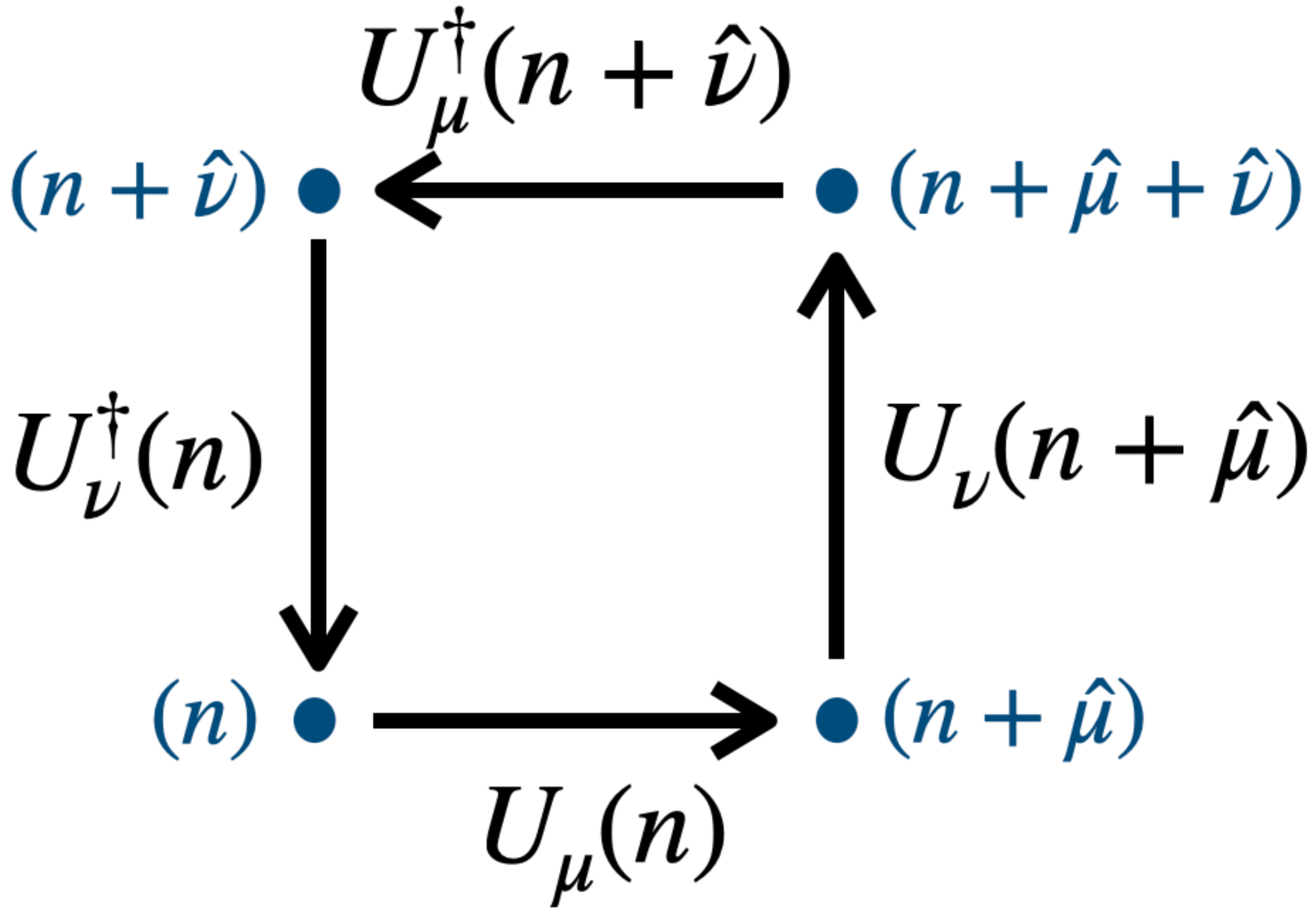
From particle data group

Lattice QCD (+ QED)

Standard perturbative techniques can't be used at low energy, the most common technique is **lattice discretization**: the theory is defined on a space-time lattice. The fields entering the action are:

- ψ_f : fermion fields defined on lattice sites
- U^a_μ: strong gauge fields, defined on links between sites and used to build the plaquette (fundamental gauge quantity on the lattice)
- A_μ: electromagnetic field, defined on links between sites





Lattice QCD (+QED)

Lattice spacing is the fundamental unit length and all the observables measured on the lattice are **dimensionless**, because they can be expressed as a function of the lattice spacing. One observable need to be used to **fix the scale**.

$N_f + 1 + 1$ observable are used to fix the parameters of the theory: N_f quark masses, the strong coupling β and the (EM) fine structure constant α.

Lattice QCD (+QED)

Knowing the discretized Lagrangian L of the theory, it is possible to define the euclidean path integral formulation:

$$Z = \mathrm{Tr}\left[e^{-\beta H}\right] \rightarrow Z = \int d\phi \exp\left[-\int d^4x\, L\right] = \int d\phi\; e^{-S}$$

Monte-Carlo simulations can be performed on a finite lattice in order to simulate the value of the fields ϕ_n at each step n of the simulation and compute observables as:

$$\langle O(x) \rangle = \sum_n \frac{O\left[\phi_n(x)\right] e^{-S(\phi_n)}}{Z}$$

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QCD (+QED) ensembles

Some lattice QCD terminology:

- **Configuration:** Collection of the values of all fields defined on the space-time lattice at a certain step of the Markov chain (intermediate steps of the simulation)
- **Ensemble:** Collection of configurations with the same physical parameters. Since QCD is a non-perturbative theory the ensemble is our description of the quantum vacuum of the theory, where observables can be measured

QCD (+QED) simulations

Scheme of a lattice simulation:

1. Tuning
2. Ensemble production
3. Measurement of observables
4. Statistics

C* boundary conditions

Consists in the charge conjugation of both gauge and fermionic fields at the boundary:

- U(1) gauge links: $$U_\mu(x + L\hat{k}) = U_\mu^*(x)$$
- Fermion fields: $$\psi_f(x + L\hat{k}) = C^{-1}\overline{\psi}_f^T(x)$$

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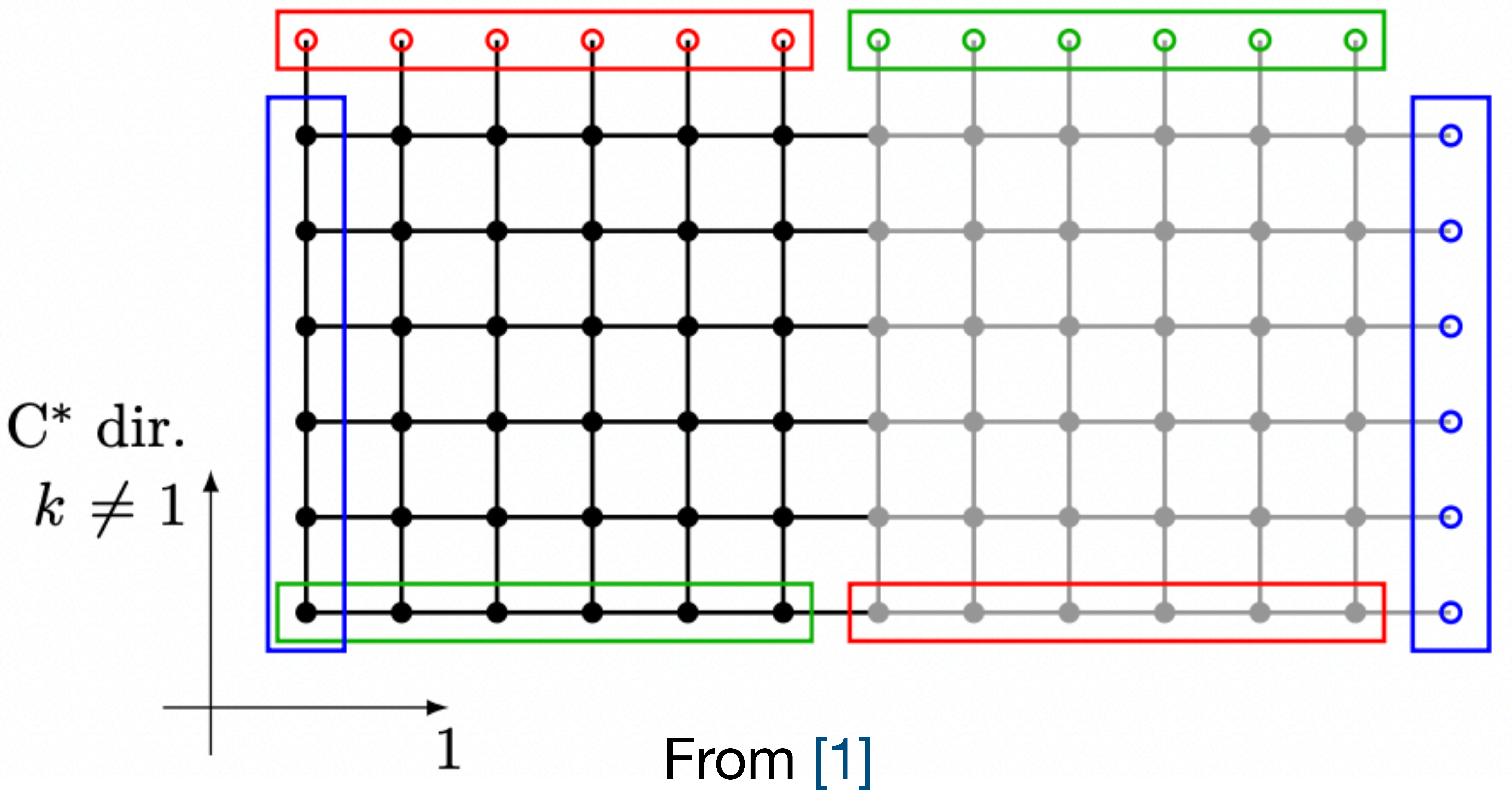
C* boundary conditions



From [1]

[1]: Isabel Campos et al. “openQ*D code: a versatile tool for QCD+QED simulations”. In: The European Physical Journal C (Mar. 2020).

Simulations with C* boundary conditions

- **Locality**: there are not any non local constraints imposed, so locality is automatically preserved

- **Gauge invariance**: can identify an expression for the U(1) gauge transformations that is invariant under charge conjugation

- **Translational invariance**: the Lagrangian is invariant under charge conjugation so it remains invariant under translations

- **Simulations and tuning are more expensive than in QCD**

HPC resources

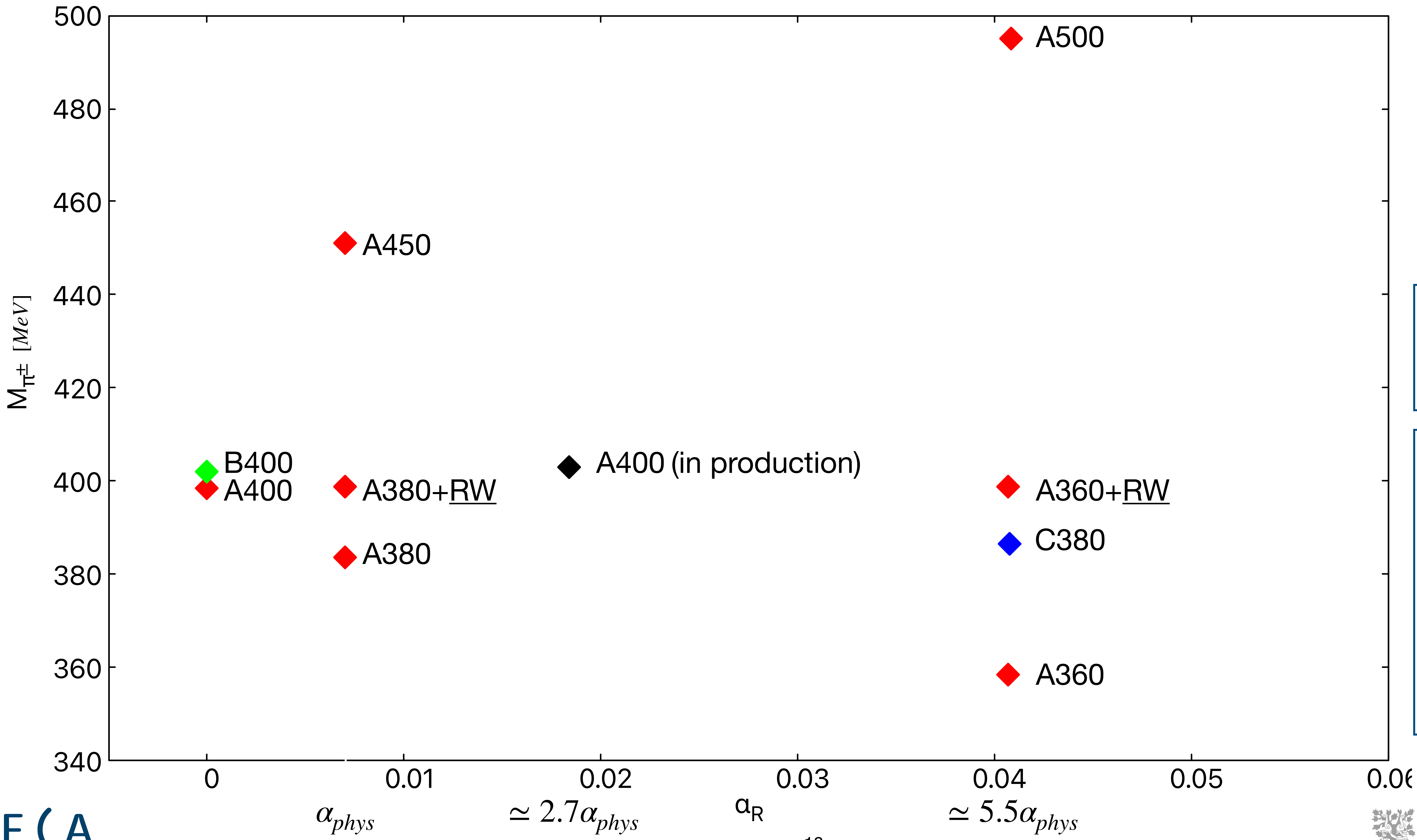
- Supercomputer Lise and Emmy at NHR@ZIB and NHR@Göttingen (**60 Millions cpu hours**)
- Marconi supercomputer (CINECA) (**10 Millions cpu hours**)
- Piz Daint (Swiss National Supercomputing Centre) (**10 Millions cpu hours**)
- Poznan Supercomputing and Networking Center (PSNC) (**20 Millions cpu hours**)

Example: Production of an ensemble at a new value of α

2048 cores, 1.3 GB per configuration

For 2000 configuration $\simeq$ 2 month, 2.6 TB

Ensembles



$a \simeq 0.054$ fm

$\beta = 3.24$

Nf = 1 + 2 + 1
u,d/s, c quarks

A = 64×32^3

B = 80×48^3

C = 96×48^3

Tuning

The target point is fixed with ϕ observables (combination of meson masses):

$$\phi_0 = 8t_0 \left(M^2_{K^\pm} - M^2_{\pi^\pm}\right) = 0$$

$$\phi_1 = 8t_0 \left(M^2_{\pi^\pm} + M^2_{K^\pm} + M^2_{K^0}\right) = 2.11$$

$$\phi_2 = 8t_0 \left(M^2_{K^0} - M^2_{K^\pm}\right) \alpha_R^{-1} = 2.36$$

$$\phi_3 = \sqrt{8t_0} \left(M_{D_s^\pm} + M_{D^0} + M_{K^0}\right) = 12.1$$

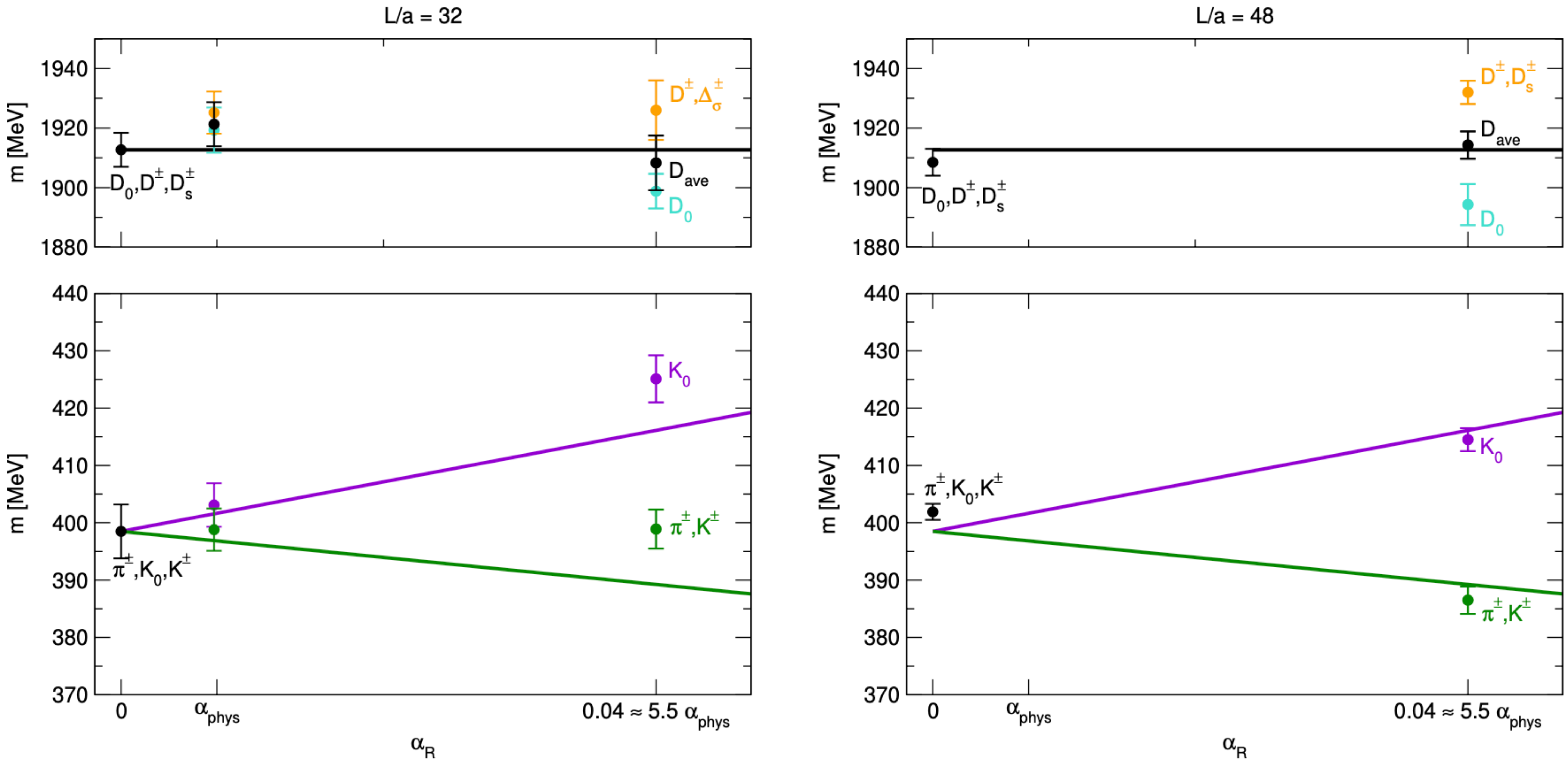
These combinations are sensitive to some combinations of the quarks masses:

- ϕ_0 is sensitive to the strange/down mass difference
- ϕ_1 is sensitive to the average of the light-quark masses as long as α_R is constant
- ϕ_2 is sensitive to the ratio between strong and electromagnetic isospin-breaking effects
- ϕ_3 essentially to fixes the charm quark mass

Meson masses: lines of constant physics

- Simulations at unphysical U-symmetric point: up, degenerate down and strange, charm quarks

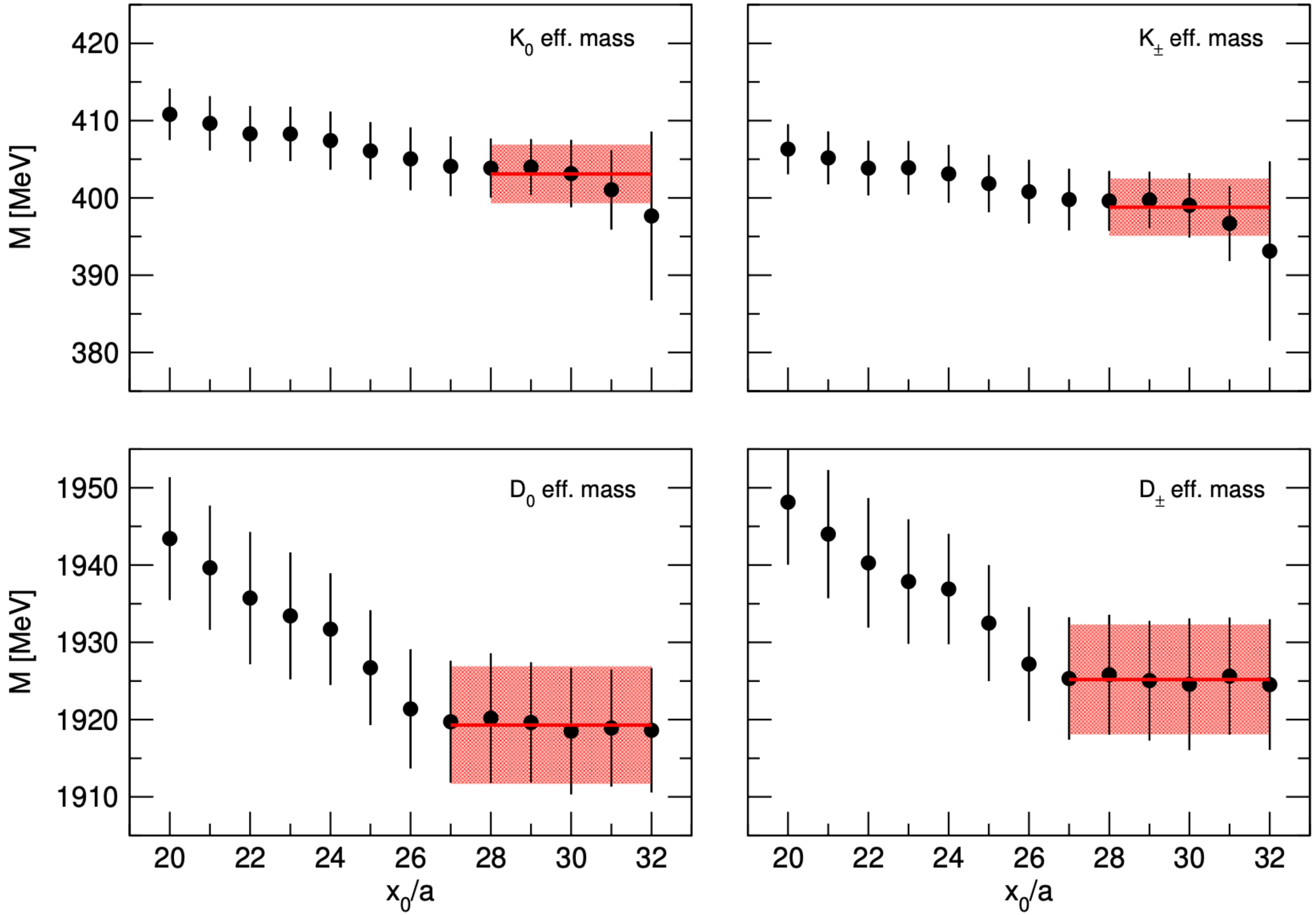
- Degenerate K and Π meson: $M_{\pi^{phys}} < M_\pi = M_K < M_{K^{phys}}$



From [2]: meson effective masses

[2]: Lucius Bushnaq et al. First results on QCD+QED with C* boundary conditions. In: Journal of High Energy Physics 2022

Meson masses



$$\lim_{t \to +\infty} C(t) = C_0 e^{-M_{had}\, t}$$

[2]: Lucius Bushnaq et al. First results on QCD+QED with C* boundary conditions. In: Journal of High Energy Physics 2022

From [2]: Meson effective masses for $\alpha = 0.05$ and volume 64×32^3

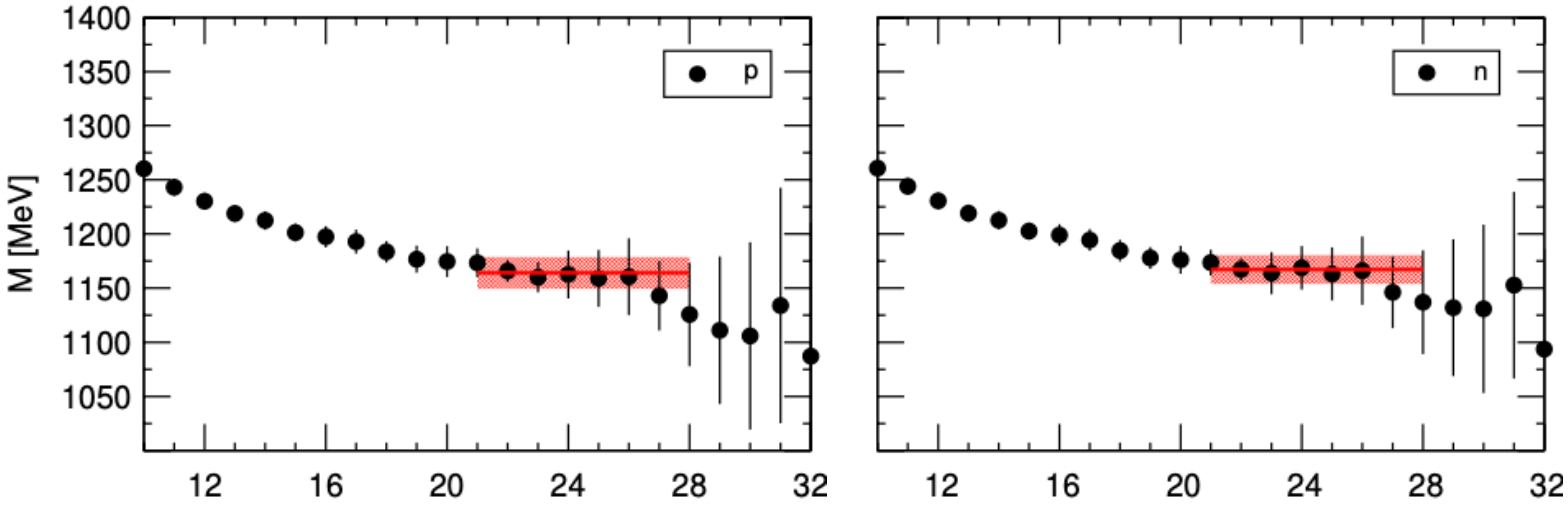
Baryon masses: signal to noise ratio problem

Signal to noise ratio (StN) : measures the clarity of the signal compared to the noise.

Baryon masses are more difficult to compute than meson masses due to the **signal to noise ratio problem**: the signal decades exponentially relatively to the noise.

$$StN(C_i) \sim \frac{\langle C_i \rangle}{\sqrt{\langle |C_i|^2 \rangle}} \sim e^{-(M_N - \frac{3}{2} m_\pi)t}$$

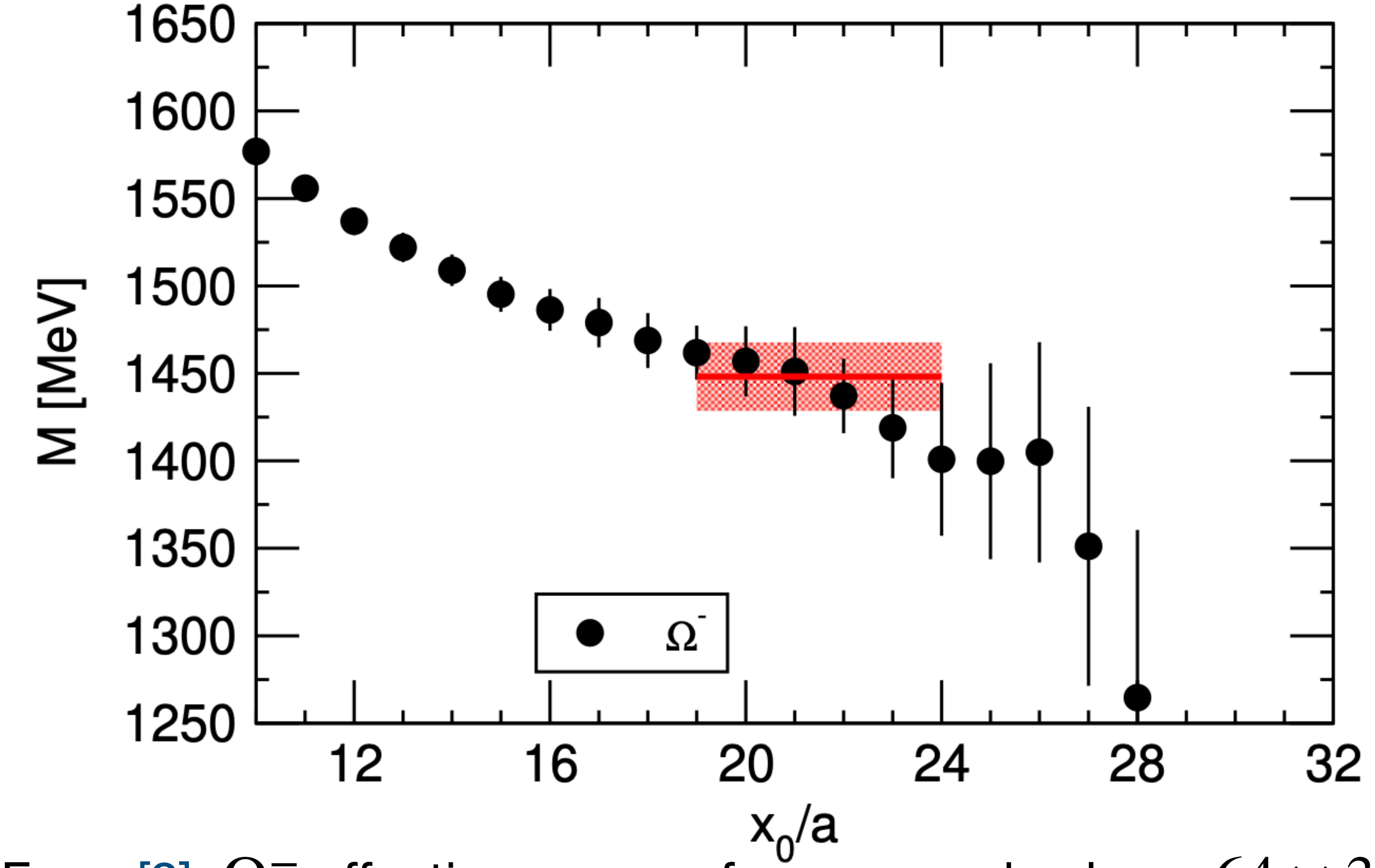
Baryon masses: p-n



From [2]: p and n effective masses for α_{phys} and volume 64×32^3

[2]: Lucius Bushnaq et al. First results on QCD+QED with C* boundary conditions. In: Journal of High Energy Physics 2022

Baryon masses: Ω^-



From [2]: Ω^- effective masses for α_{phys} and volume 64×32^3

[2]: Lucius Bushnaq et al. First results on QCD+QED with C* boundary conditions. In: Journal of High Energy Physics 2022

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Future objectives

- Baryon masses (Ω^- baryon for scale setting): add additional contributions due to C* boundary conditions vanishing in the infinite volume limit and implement noise reduction techniques

- $N_f = 1 + 1 + 1 + 1; \qquad m_u \neq m_d \neq m_s \neq m_c$

- Moving towards physical meson masses (lighter pions and heavier kaons)

Thanks for your attention

QCD + QED at finite volume

Other possibilities: QED_L and QED_M

- QED_L : non local constraint

$$\int dx^3 A_\mu = 0$$

- QED_M: massive photon

Other strategy for the simulations:

- Rome123 method: expansion of the observables in powers of e, $\delta\beta = O(e^2)$ and $\delta m = O(e^2)$

Details on QCD+QED on the lattice

- Compact formulation of QED: use of gauge links instead of vector potential. To preserve gauge invariance because this formulation doesn't need gauge fixing.

- Gauge invariant interpolating operators: string operator

$$\Psi_s(x) = e^{-\frac{iq}{2}\int_{-x_k}^{0} ds\, A_k(x+s\hat{k})}\ \psi(x)\ e^{\frac{iq}{2}\int_{0}^{L-x_k} ds\, A_k(x+s\hat{k})}$$

Details on QCD+QED on the lattice

- Coupling of the fermion field to the photon field:

$$D[U^2] = m + \frac{1}{2}\sum_{\mu=0}^{3}\left[\gamma_\mu\left(\nabla_\mu^*[U^2] + \nabla_\mu[U^2]\right) - \nabla_\mu^*[U^2]\nabla_\mu[U^2]\right]$$

$$\nabla_\mu[U^2]\psi(x) = U(x,\mu)^2\psi(x+\hat{\mu}) - \psi(x)$$

So that the string operator is local (doesn't involve taking the equivalent of a square root of the U(1) gauge links).

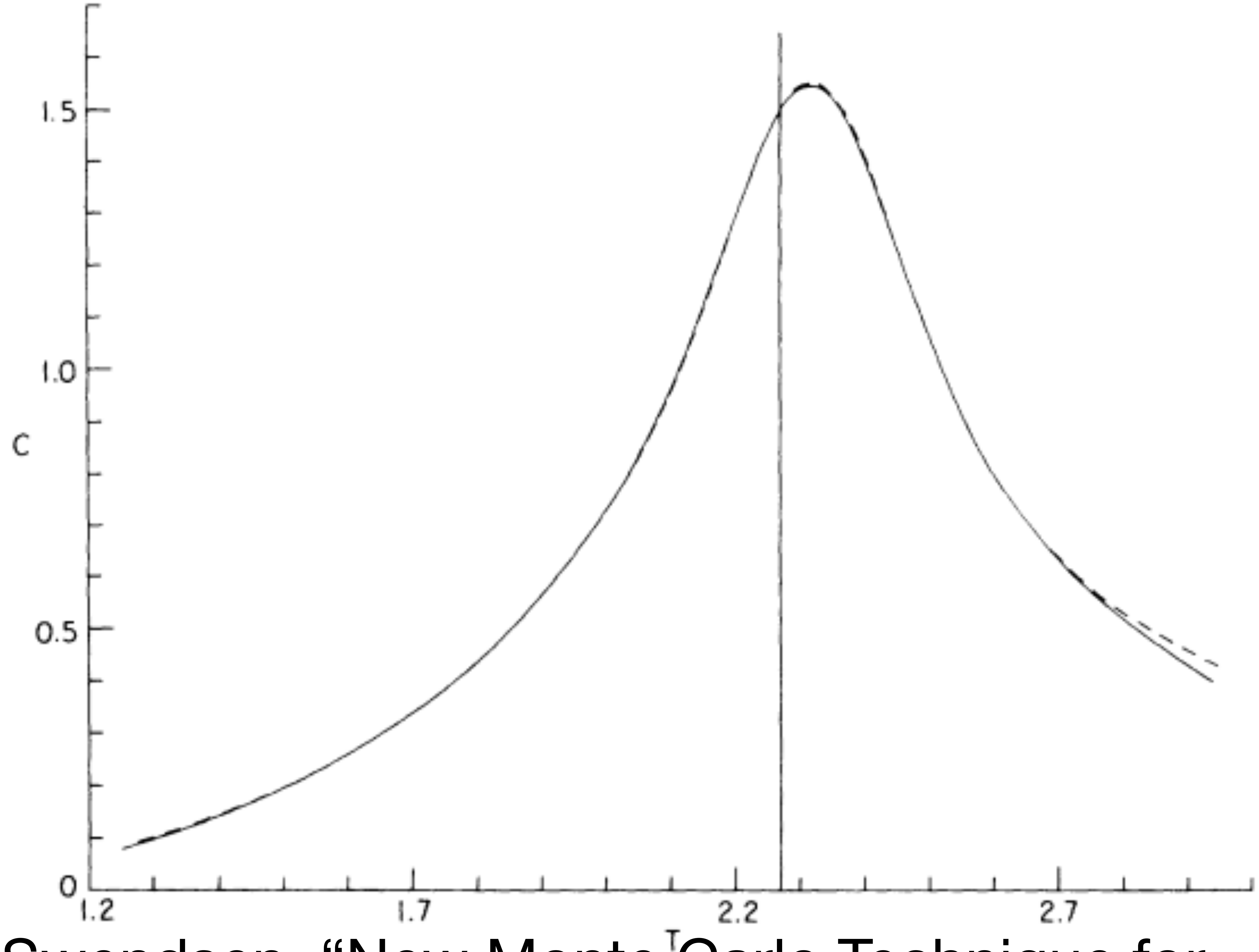
When adding QCD we have to take into account that the couplings of the quark fields to the EM fields are $q_f = -\frac{1}{3}, \frac{2}{3}$, the Dirac operator is then obtained doing the substitution:

$$U^2 \rightarrow U^{6q_f}$$

Ensembles: mass reweighting

The idea of reweighting for Monte Carlo simulation was first introduced in [3] in the case of statistical physics, on a case study of the 2D Ising model.

With this technique, starting from a simulation at fixed parameters, it is possible to scan a region of parameters close to the simulated one, (phase transition region).



[3]: Alan M. Ferrenberg and Robert H. Swendsen. "New Monte Carlo Technique for Studying PhaseTransitions". In: Physical Rewiew Letters (Dec. 1988)

Ensembles: mass reweighting

In the case of mass reweighting for lattice gauge theories from a simulation at fixed parameters it is possible to obtain observables at different values of the quark masses.

O that does not explicitly depend on the quark masses:

$$< O >_t = \frac{< OW(m_t, m_i) >_i}{< W(m_t, m_i) >_i}$$

O that explicitly depends on the quark masses:

$$< O(m_t) >_t = \frac{< O(m_t)W(m_t, m_i) >_i}{< W(m_t, m_i) >_i}$$

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