

## Introduction

- The Standard Model describes all basic particles and the basic forces, electroweak and strong.
- Quantum Chromodynamics (QCD)** describes how particles behave under the strong force
- “Chromo”** stands for the color charge (RGB) that the quarks and gluons carry
- Only quarks and gluons interact via the strong force
- The strong force is the force that holds together particles such as pions, protons, and neutrons
- Our simulation only includes **2+1** quarks, the **up (u)**, **down (d)**, and **strange (s)**

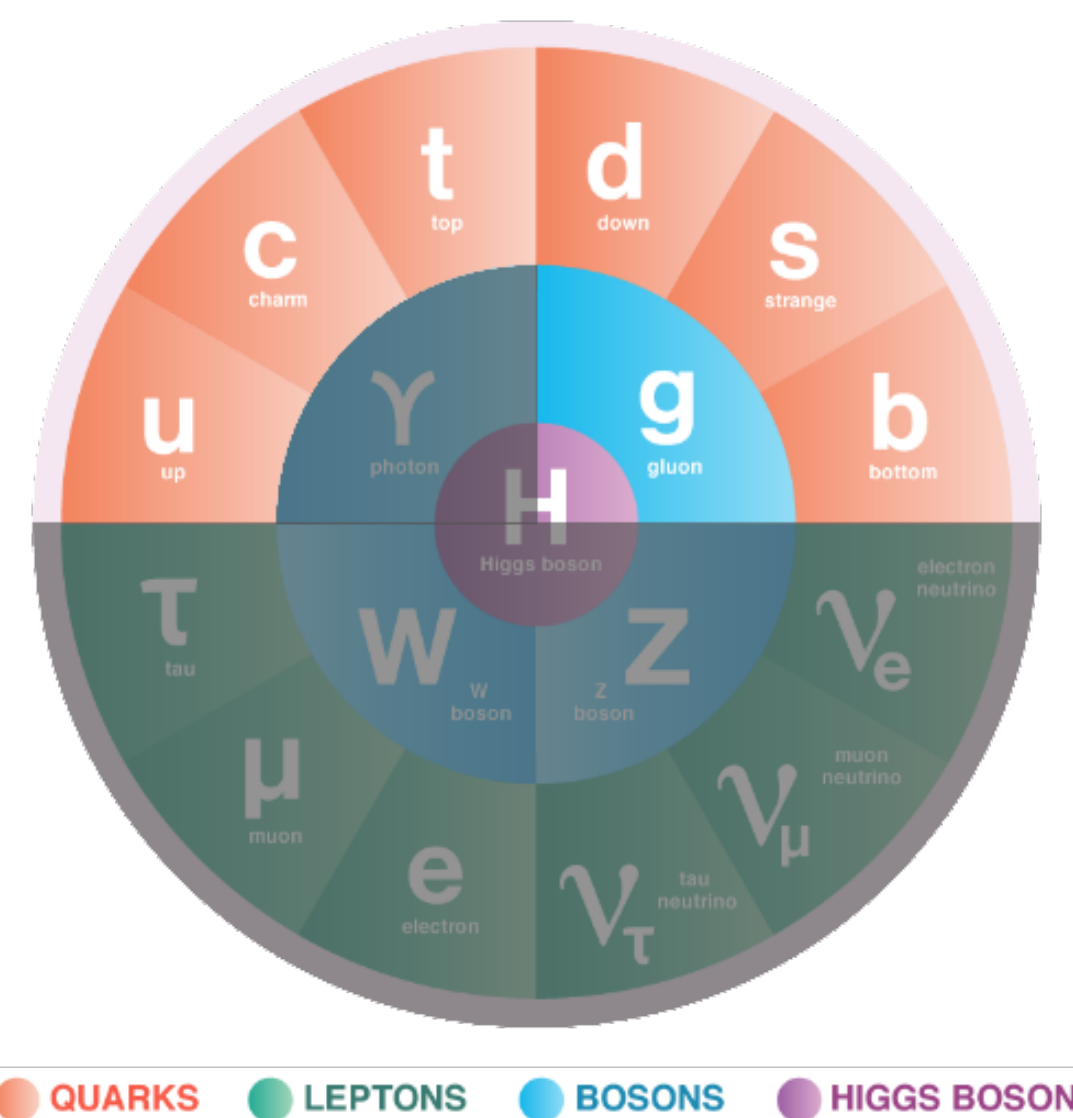


Figure 1. Particles in the Standard Model. Strong force particles are unshaded (does not include Higgs boson) [1].

## $N_\pi$ Scattering: A Delta Resonance

Our results focus on nucleon-pion scattering where the nucleon can be a proton or neutron. We look at all interactions where

$$N \pi \longrightarrow N \pi$$

Different variations of this interaction are called channels. One such channel contains a delta resonance, where a delta particle is created and then decays back into a nucleon pion pair.

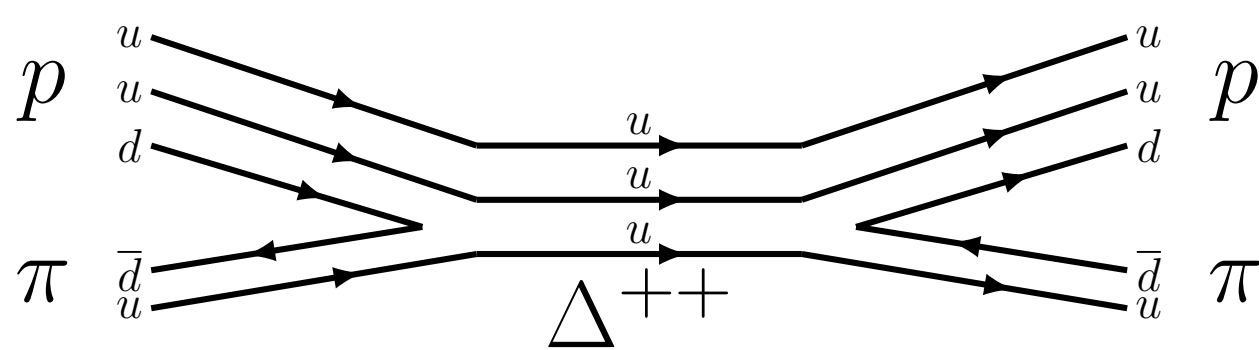


Figure 2. Proton ( $p$ ) and pion ( $\pi$ ) scattering with a delta ( $\Delta$ ) resonance example.

## Simple Harmonic Oscillator Toy Model

To demonstrate the methodology to calculate the energy spectrum from first principles physics, we will begin with a toy model: a 1D simple harmonic oscillator (SHO).

An SHO example: think of the movement of a pendulum viewed from above.

### First principle physics: Lagrangian of SHO:

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2 \quad (1)$$

where  $x$  is the position of mass  $m$ ,  $\dot{x} = \frac{dx}{dt}$ , and  $\omega$  is the angular frequency. A Lagrangian describes the dynamics of the system using the energies,  $L = \text{kinetic energy} - \text{potential energy}$ .  $t$  is time.

## References

- <sup>1</sup>The standard model of particle physics, <https://www.symmetrymagazine.org/standard-model/>.
- <sup>2</sup>G. S. Bali, E. E. Scholz, J. Simeth, and W. Söldner (RQCD), “Lattice simulations with  $N_f = 2+1$  improved Wilson fermions at a fixed strange quark mass”, Phys. Rev. D **94**, 074501 (2016).
- <sup>3</sup>M. Bruno et al., “Simulation of QCD with  $N_f = 2 + 1$  flavors of non-perturbatively improved Wilson fermions”, JHEP **02**, 043 (2015).
- <sup>4</sup>Juqueen, [https://web.archive.org/web/20190118115058/https://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUQUEEN/JUQUEEN\\_node.html](https://web.archive.org/web/20190118115058/https://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUQUEEN/JUQUEEN_node.html).
- <sup>5</sup>Texas advanced computing center, <https://www.tacc.utexas.edu/systems/frontera>.
- <sup>6</sup>M. Lüscher, <https://luscher.web.cern.ch/luscher/openQCD/>.
- <sup>7</sup>C. Morningstar, J. Bulava, B. Fahy, J. Foley, Y. C. Jhang, K. J. Juge, D. Lenkner, and C. H. Wong, “Extended hadron and two-hadron operators of definite momentum for spectrum calculations in lattice QCD”, Physical Review D **88**, 10.1103/physrevd.88.014511 (2013).

## SHO Energy Spectrum from Monte Carlo

In classical mechanics, there is one path from point  $(x_a, t_a)$  to  $(x_b, t_b)$ , but for quantum mechanics, a particle can take any path. In Monte Carlo, we use random numbers to simulate these possible paths.



The quantum mechanics for a system can be characterized by the transition amplitude that determines the probability that starts at point  $(x_a, t_a)$  and ends at  $(x_b, t_b)$  by integrating over all possible paths with phase amplitude  $\exp(iS/\hbar)$

$$Z(b, a) = \int_a^b \mathcal{D}x e^{iS/\hbar} \xrightarrow{t \rightarrow -i\tau} \int_a^b \mathcal{D}x e^{-S/\hbar} \quad (2)$$

where  $S$  is the action  $S = \int_{t_a}^{t_b} L dt$ . Under a Wick rotation of time ( $t \rightarrow -i\tau$ ), this phase turns into a weight, i.e. each path has a probability  $\exp(-S/\hbar)$  to occur. To see how different paths contribute to the transition probability, several paths are mapped out on a lattice in the  $\tau$  domain in Figure 3.

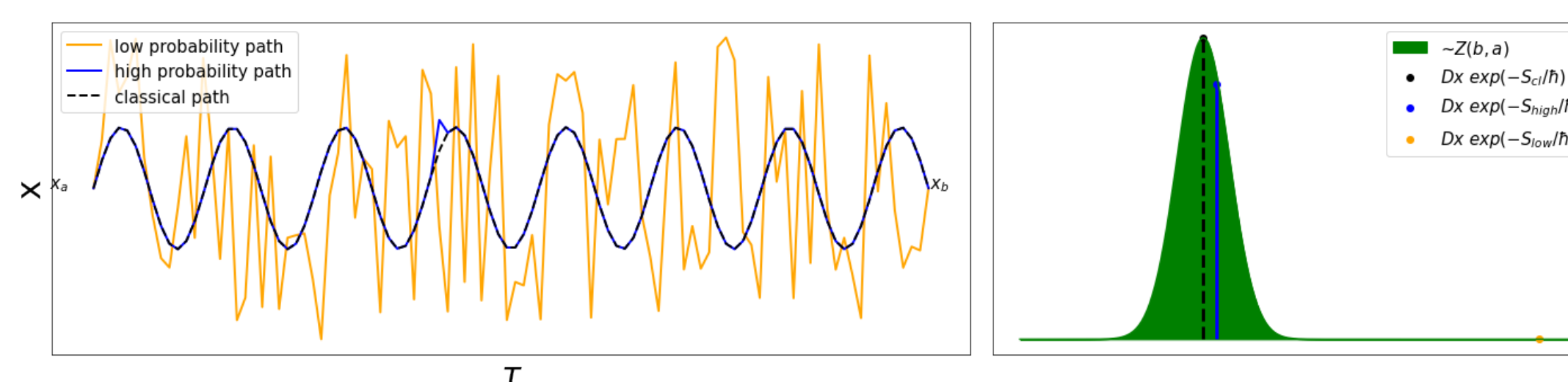


Figure 3. A few paths and their contribution to the transition amplitude. Available at qrd.by/sho.

To capture the quantum physics, we want to generate paths that are primarily in the peak of the transition amplitude, so we use the Metropolis-Hastings method to choose the paths/configurations. A few configurations are shown out in Figure 4.

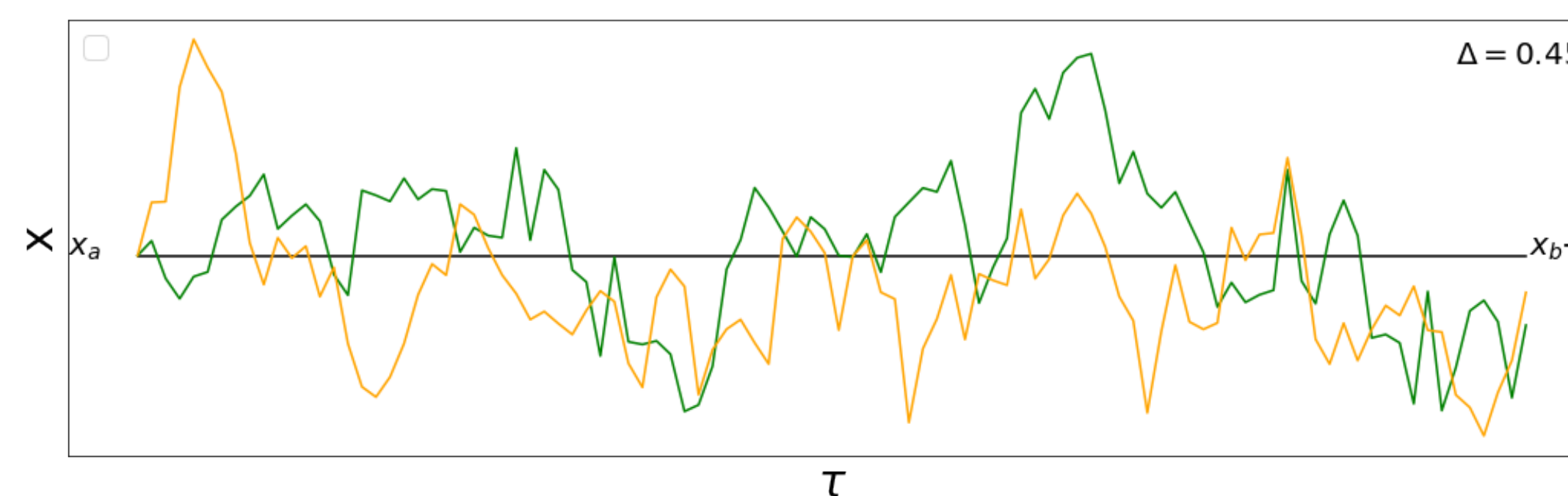


Figure 4. Configurations computed using the Metropolis-Hastings method. Available at qrd.by/sho.

Using these configurations, we can calculate correlation functions,  $\langle \phi_0 | x(\tau) x(0) | \phi_0 \rangle$ . These correlations functions can be related to the energies  $E_n$  of the system using spectral analysis with overlap amplitude  $A_n$ .

$$\langle \phi_0 | x(\tau) x(0) | \phi_0 \rangle = \sum_{n=0}^{\infty} A_n^2 \exp\left(\frac{-(E_n - E_0)\tau}{\hbar}\right) \quad (3)$$

Using this relation, we can fit to the lowest lying energy spectrum.

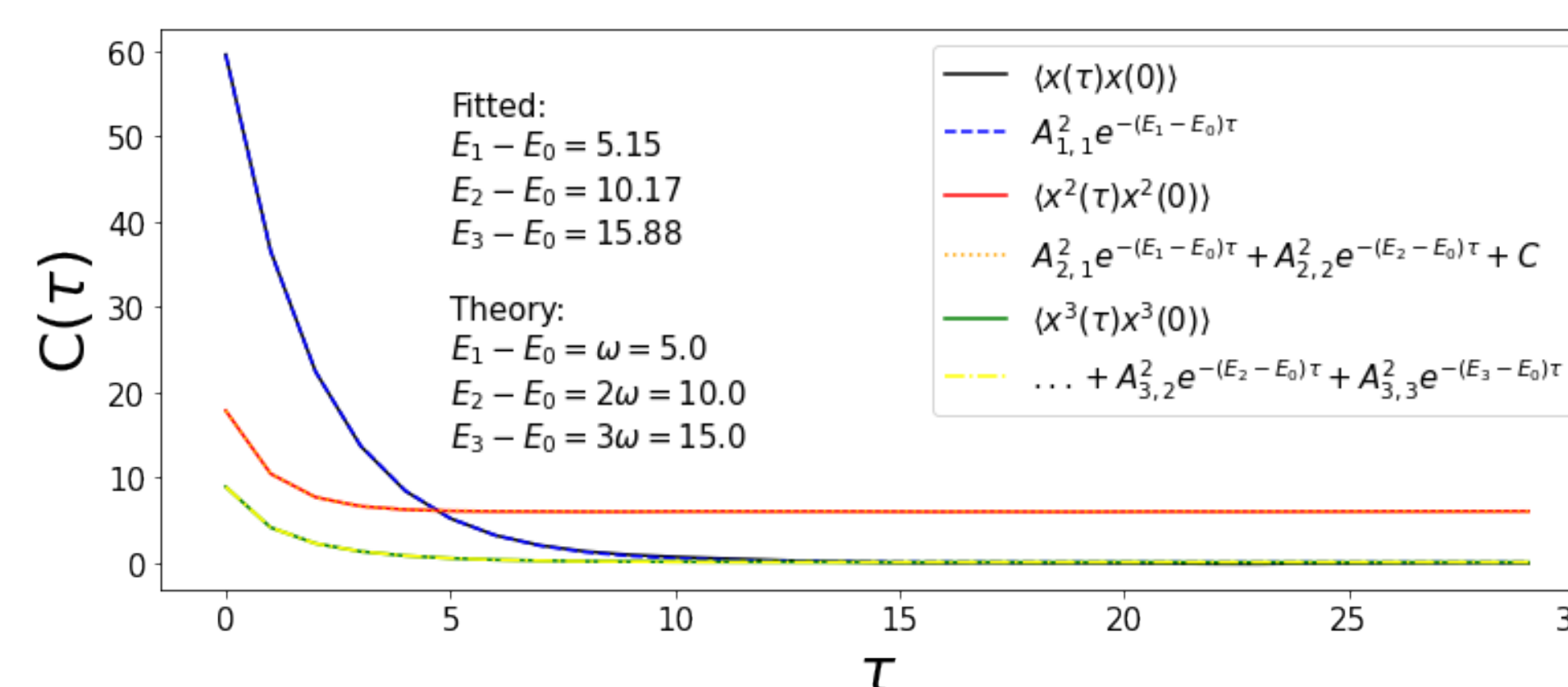


Figure 5. Several fitted correlation functions produced from SHO Example repository (qrd.by/sho). The fit results are compared to analytical calculations.  $\hbar = c = 1$

## Lattice QCD

QCD Lagrangian density ( $L = \int d^3x \mathcal{L}$ ):

$$\mathcal{L}[\psi, \bar{\psi}, A] = \sum_{f=1}^{N_f} \bar{\psi}_{a\alpha}^{(f)} (i\gamma_{\alpha\beta}^{\mu} \mathcal{D}_{\mu ab} - m^{(f)} \delta_{\alpha\beta} \delta_{ab}) \psi_{a\alpha}^{(f)} - \frac{1}{4} G_{\mu\nu}^a G_{\mu\nu}^a, \quad (4)$$

$$\mathcal{D}_{\mu} = \partial_{\mu} + ig\mathcal{A}_{\mu}; \quad G_{\mu\nu} = -\frac{i}{g}[\mathcal{D}_{\mu}, \mathcal{D}_{\nu}]; \quad \mathcal{A}_{\mu} = \mathcal{A}_{\mu}^a \frac{\lambda_a}{2} \quad (5)$$

- $\psi, \bar{\psi}$  – fermionic quark fields, Dirac spinors with mass  $m$  and flavor  $f$
- $\mathcal{A}_{\mu}$  – gluon fields, non-abelian, SU(3) symmetry described by Gell-Mann matrices  $\lambda$
- $\gamma^{\mu}$  – Dirac gamma matrices
- $g$  – coupling strength
- fermionic color indices  $a, b = 1, 2, 3$
- gluonic color indices  $a = 1, 2, \dots, 8$
- Dirac indices  $\alpha, \beta = 1, 2, 3, 4$
- Minkowski space-time indices  $\mu, \nu = 1, 2, 3, 4 - x, y, z, t$

### Changes from SHO to QCD:

- QCD is 4D - 3 spacial dimensions and 1 time dimension
- QCD is a gauge theory, adds constraints to the degrees of freedom
- for every flavor of quark there are 2 corresponding 12-vector fields  $\psi, \bar{\psi}$
- there are 8 gluon fields

To retrieve the energy spectrum, we use hadronic annihilation operators in our time-ordered 2-point correlator in natural units ( $\hbar = c = 1$ ):

$$C_{ij}(t) = \langle 0 | T \mathcal{O}_i(t + t_0) \bar{\mathcal{O}}_j(t_0) | 0 \rangle = \sum_n \langle 0 | \mathcal{O}_i | n \rangle \langle n | \bar{\mathcal{O}}_j | 0 \rangle e^{-(E_n - E_0)t} \quad (6)$$

where hadronic operators can represent the individual particles  $N, \pi$ , or the combined  $N\pi$  system.

## Results and Conclusions: $N\pi$ Energy Spectrum

Parameters of the D200 ensemble produced by the Coordinated Lattice Simulation Group can be found in Refs. [2, 3]. Configurations were calculated on JUQUEEN [4], and correlators on Frontera [5]. openQCD was used for many calculations [6].

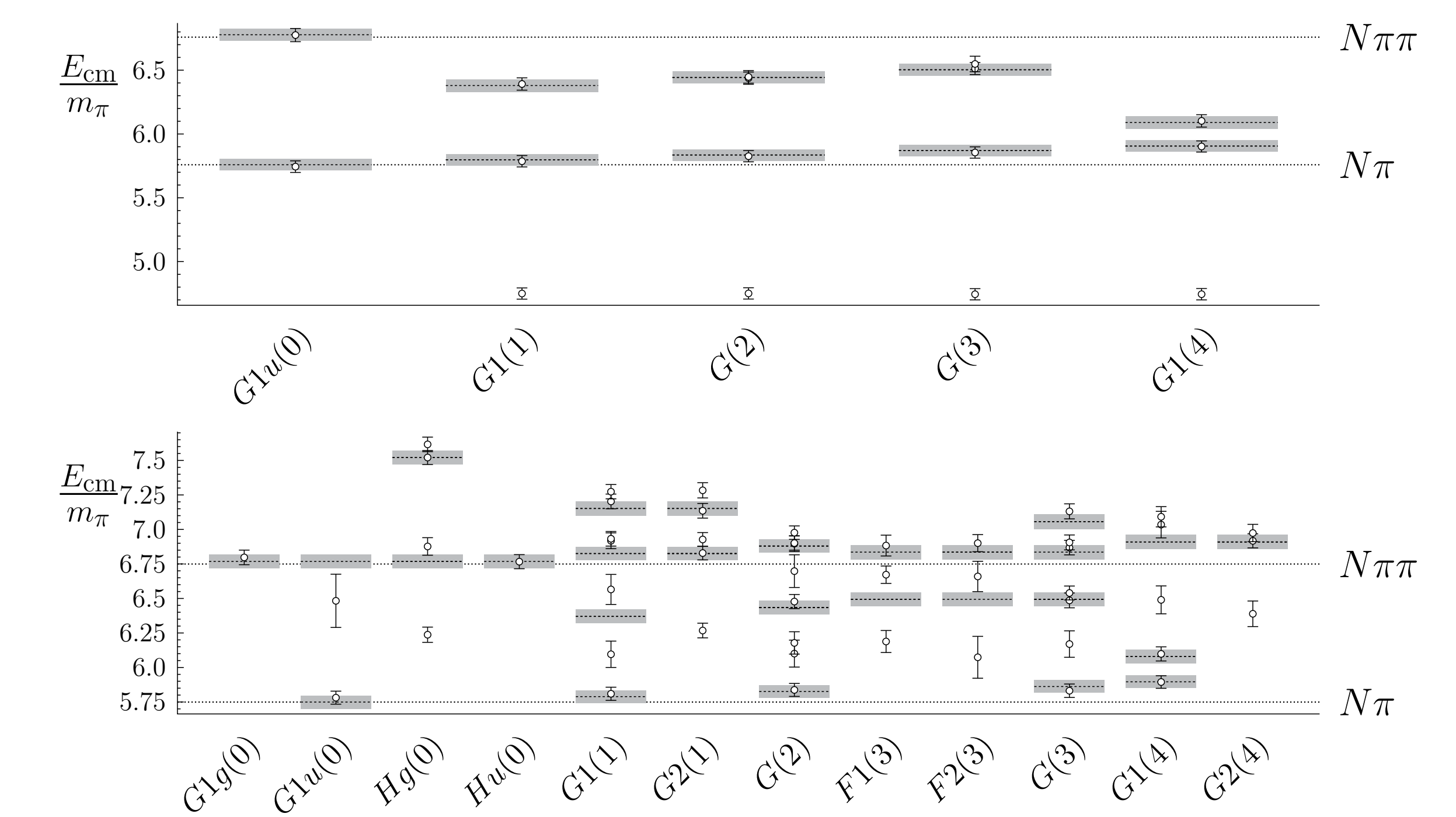


Figure 6. Top:  $I = 1/2$ . Bottom:  $I = 3/2$ . The notation along the horizontal axis is  $\Lambda(\mathbf{P}^2)$ , where  $\mathbf{P}^2$  is the total momentum squared and  $\Lambda$  is the irrep of little group  $\mathbf{P}$  [7]. Dashed lines indicate the limits of the elastic region. Solid lines and shaded regions indicate the non-interacting levels and their errors.

The  $N\pi$  channels that we study here are also known as the roper and delta resonance channels. We can see evidence of resonances when the energy spectrum differs from the non-interacting spectrum. Though we don't see this behavior in the  $I = 1/2$  channel, we do see evidence of delta resonance in  $I = 3/2$  channel. Using this data, we can investigate the delta resonance, which is needed information for the Deep Underground Neutrino Experiment ([www.dunescience.org](http://www.dunescience.org)).