QCD: Numerical integration of a Quantum Field Theory

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Integrability, Anomalies and Quantum Field Theory, IHÉS, February 2020

20 years (nearly) with Samson at TCD

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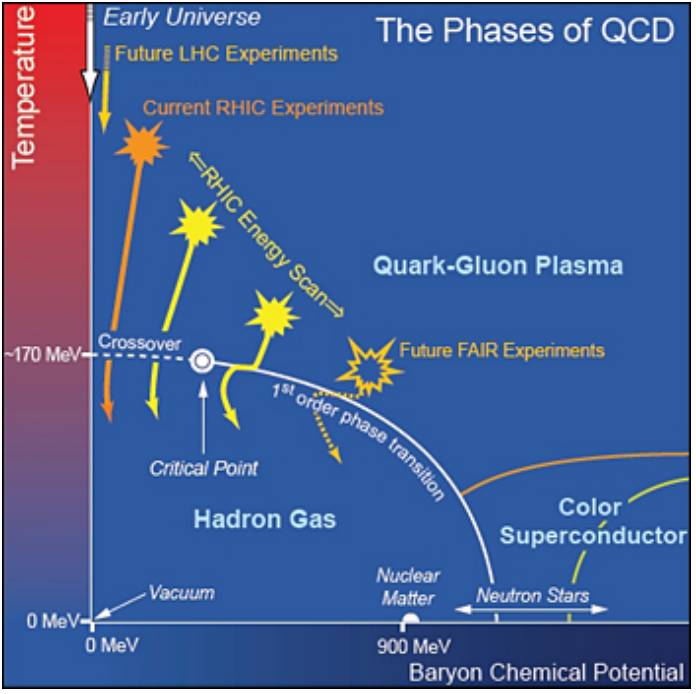
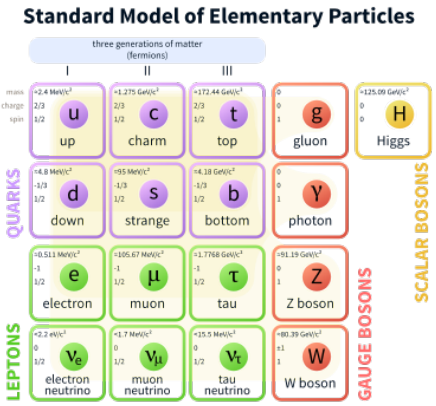
Some Rubrics history!
"In 1732 a group of students, particularly annoyed with a fellow of the college did what all rational types do and gathered a mob outside his window and shot him."
A more peaceful environment these days .... mostly ...

Lattice QCD
methods, progress & challenges


The Phases of QCD
Temperature
Early Universe
Future LHC Experiments
Current RHIC Experiments
⇐RHIC Energy Scan⇒
Quark-Gluon Plasma
Future FAIR Experiments
~170 MeV
Crossover
1st order phase transition
Critical Point
Hadron Gas
Color Superconductor
Nuclear Matter
Neutron Stars
Vacuum
0 MeV
0 MeV
900 MeV
Baryon Chemical Potential

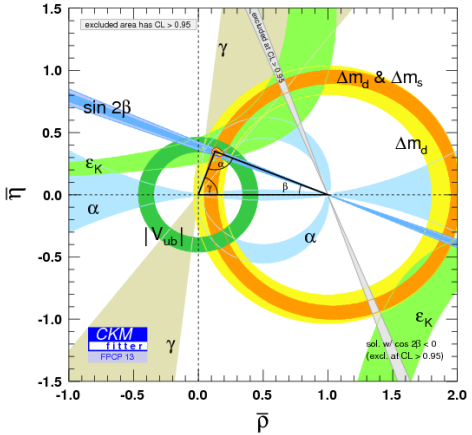
Quantum ChromoDynamics - the theory of quarks and gluons

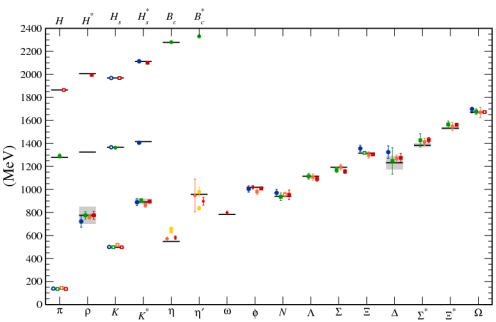


- Embarassingly successful
- Precision tests of SM can reveal new physics - more important than ever!

- **QCD is the only experimentally studied strongly-interacting quantum field theory - highlights many subtleties.**
- **A paradigm for other strongly-interacting theories in BSM physics.**
- **There are still puzzles and surprises in this well-studied arena.**

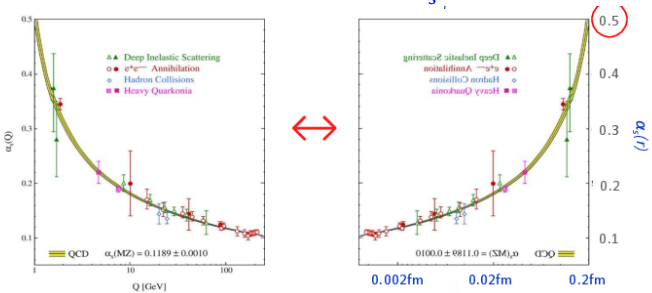
(Lattice) QCD for phenomenology





A tale of two regimes

A running coupling $\alpha_s = g_s^2/(4\pi)$



High Energy

- asymptotic freedom, perturbative
- degrees of freedom: quarks & gluons

Low Energy

- nonperturbative, $\Lambda_{\mathrm{QCD}} \sim 300MeV = \mathcal{O}(1fm^{-1})$
- color confinement, degrees of freedom: mesons & baryons

Theory of quarks & gluons $\longrightarrow$ low-energy hadron spectrum

Why Lattice QCD ?

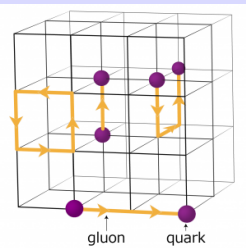
- A systematically-improvable non-perturbative formulation of QCD
  - Well-defined theory with the lattice a UV regulator
- Arbitrary precision is in principle possible
  - of course algorithmic and field-theoretic complications can make this challenging!
- Starts from first principles - i.e. from the QCD Lagrangian
  - inputs are quark mass(es) and the coupling - can explore mass dependence and coupling dependence but getting to physical values can be hard!

A lattice QCD primer

Start from the QCD Lagrangian:

$$\mathcal{L} = \bar{\psi}\left(i\gamma^\mu D_\mu - m\right)\psi - \tfrac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a$$

- Gluon fields are SU(3) matrices - links of a hypercube.
  $A_\mu(x) \rightarrow U_\mu(x) = \mathcal{P} e^{ig\int_x^{x+e\mu} dz_\mu A_\mu(z)}$
- Quark fields $\psi(x)$ on sites with color, flavor, Dirac indices.
  Fermion discretisation - Wilson, Staggered, Overlap.
- Derivatives $\rightarrow$ finite differences:
  $\nabla^{\text{fwd}}_\mu \psi(x) = \frac{1}{a}\left[U_\mu(x)\psi(x + a\hat{\mu}) - \psi(x)\right]$



Solve the QCD path integral on a finite lattice with spacing $a \neq 0$ estimated stochastically by Monte Carlo. Can only be done effectively in a Euclidean space-time metric (no useful importance sampling weight for the theory in Minkowski space).
Observables determined from (Euclidean) path integrals of the QCD action

$$\langle \mathcal{O} \rangle = 1/Z \int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \; \mathcal{O}[U, \bar{\psi}, \psi] e^{-S[U,\bar{\psi},\psi]}$$

Correlators in Lattice Euclidean Field Theory: I

- Physical observables $\mathcal{O}$ are determined from

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D}\Psi \mathcal{D}\bar{\Psi} \mathcal{O} e^{-S_{QCD}}$$

- Analytically integrate Grassman fields (Ψ, $\bar{\Psi}$) $\rightarrow$

$$\langle \mathcal{O} \rangle \overset{N_f=2}{=} \frac{1}{Z} \int \mathcal{D}U \det\left(M^\dagger(U) M(U)\right) \mathcal{O} e^{-S_G(U)}$$

  Calculated by importance sampling of gauge fields and averaging over ensembles.
- Simulate $N_{\rm cfg}$ samples of the field configuration, then

$$\langle \mathcal{O} \rangle = \lim_{N_{cfg} \rightarrow \infty} \frac{1}{N_{cfg}} \sum_{i=1}^{N_{cfg}} \mathcal{O}_i[U_i]$$

- Correlation functions have a (improvable!) statistically uncertainty $\sim 1/\sqrt{N_{cfg}}$.
- Calculating $\det M$ for M a large, sparse matrix with small eigenvalues takes $> 80\%$ of compute cycles in configuration generation. $\det M = 1$ is the quenched approximation.

Correlators in lattice Euclidean field theory: II

- We are interested in two-point correlation functions built from interpolating operators (functions of ψ):
  - Eg the local meson operator $\phi(x) = \bar{\psi}_a(x)\Gamma\psi_b(x)$
  - Γ an element of the Dirac algebra with possible displacements; a and b flavour indices

$$\mathcal{O}_{\alpha\beta} = \sum_x \bar{\psi}_\alpha(x)\psi_\beta(x) \qquad \mathcal{O}^i_{\alpha\beta} = \sum_x \bar{\psi}_\alpha(x)U_i(x)\psi_\beta(x+\hat{\imath}) \qquad \mathcal{O}^{ij}_{\alpha\beta} = \sum_x \bar{\psi}_\alpha(x)U_i(x)U_j(x+\hat{\imath})\psi_\beta(x+\hat{\imath}+\hat{\jmath})$$

- The two-point function is then

$$C(t) = \langle \phi(x)\phi^\dagger(0)\rangle = \langle \bar{\psi}_a(x)\Gamma\psi_b(x)\bar{\psi}_b(0)\Gamma^\dagger\psi_a(0)\rangle, \quad x \equiv (t,\mathbf{x}); t \geq 0$$

- Using Wick's theorem to contract quark fields replaces fields → quark propagators

$$\begin{aligned} C(t,\mathbf{x}) &= -\langle \mathrm{Tr}(M_a^{-1}(0,x)\Gamma M_b^{-1}(x,0)\Gamma^\dagger)\rangle \\ &\quad +\delta_{ab}\langle \mathrm{Tr}(\Gamma M_a^{-1}(x,x))\mathrm{Tr}(\Gamma^\dagger M_a^{-1}(0,0))\rangle \end{aligned}$$

  where the trace is over spin and colour.
- For flavour non-singlets, ($a \neq b$): $C(t,\mathbf{x}) = \langle \mathrm{Tr}(\gamma_5 M_a^{-1}(x,0)^\dagger\gamma_5\Gamma M_b^{-1}(x,0)\Gamma^\dagger)\rangle$
- Fermions in lagrangian: sea quarks → fermion determinant. Fermions in measurement: valence quarks → propagators

A recipe for lattice (meson) spectroscopy

- Construct a basis of local and non-local operators $\mathcal{O}$ o.t.f. $\bar{\Psi}(x)\Gamma D_i D_j \ldots \Psi(x)$ **that overlap onto the state of interest**.
- Build a correlation matrix of two-point functions

$$C_{ij} = \langle 0|\mathcal{O}_i \mathcal{O}_j^\dagger|0\rangle = \sum_n \frac{Z_i^n Z_j^{n\dagger}}{2E_n} e^{-E_n t}.$$

- Ground state mass from fits to $e^{-E_n t}$
- Beyond ground state: Solve generalised eigenvalue problem

$$C_{ij}(t) v_j^{(n)} = \lambda^{(n)}(t) C_{ij}(t_0) v_j^{(n)}.$$

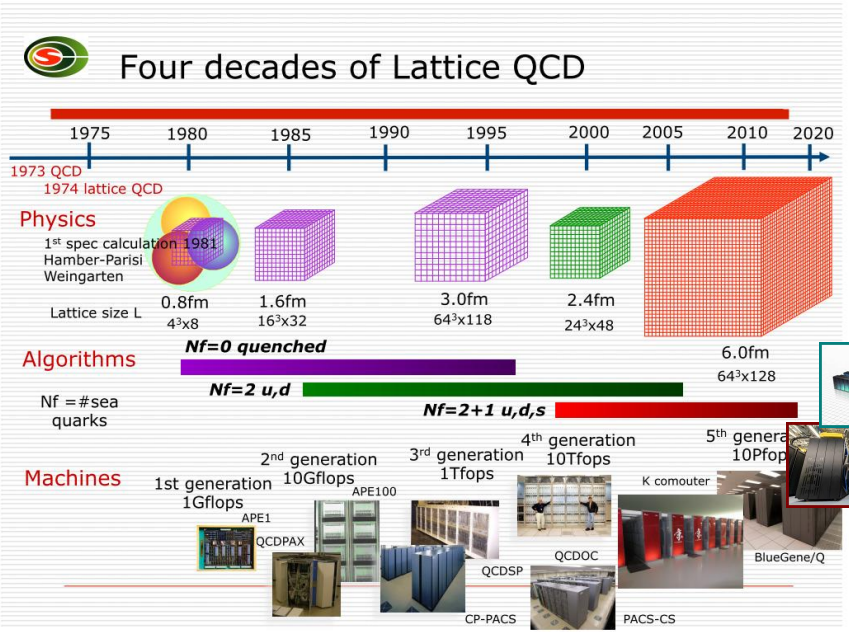
- Eigenvalues: $\lambda^{(n)}(t) \sim e^{-E_n t}\left[1 + O(e^{-\Delta E t})\right]$ - principal correlator.
- Eigenvectors: related to overlaps $Z_i^{(n)} = \sqrt{2E_n} e^{E_n t_0/2} v_j^{(n)\dagger} C_{ji}(t_0)$.

The cost of doing business

- Generating gauge ensembles at physical quark masses on large volumes requires millions of core hours.

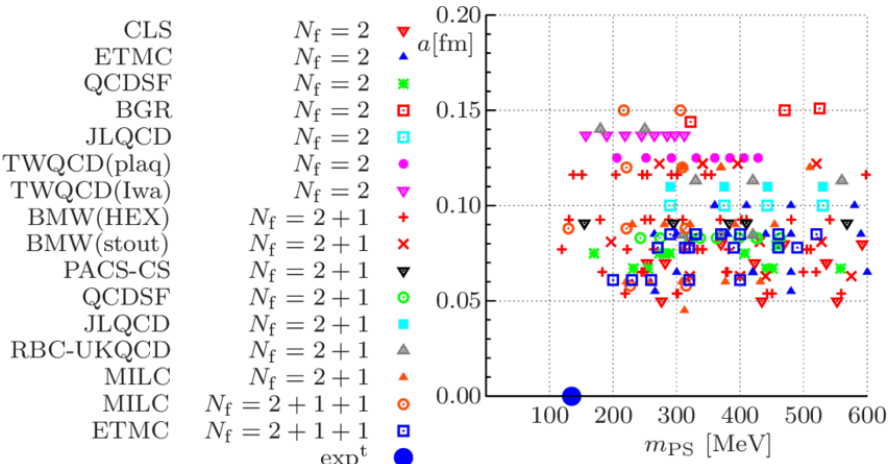
$$\text{Computational Cost} \sim c \times (\text{Number of configurations}) \times \left(\frac{1}{M_\pi}\right)^6 \times (L)^5 \times \left(a^{-1}\right)^7$$

- Once the gauge configurations are generated "just" have to invert the Dirac matrix M to get fermion propagators, with $L > 1$fm and $a << 1$ fm.
  - a lattice volume $32^4 = 1,048,576$ sites
  - a fermion (quark) has 4 Dirac components
  - 3 colours in $SU(3)$
  - $\Rightarrow M$ is easily $10^8 \times 10^8$
- Requires high memory/network bandwidth, but also highly parallelisable
- Tera/Peta bytes of data is also generated!



ETM collaboration

The lattice simulation landscape



from K. Jansen et al

Below thresholds: "gold-plated" quantities characterised by

- Using well-tried and tested and validated methods.
- High statistics and improved actions for precise results.
- Different actions in agreement.
- Most/All systematic errors accounted for e.g. continuum extrapolation, finite volume, physical light quark masses, Nf, EM effects.

Above thresholds: strong exotic matter

- Physics of molecular/multi hadron states needs relevant operators.
- No continuum extrapolation.
- Relatively heavy pions.
- Improvements underway as methods improve.

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Terra Incognita

- Finite density: Monte Carlo not valid!
- Scattering at finite temperature ...

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- …adron
- …perators.
- …xtrapolation.
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New ideas have been crucial!

- *Distillation*: 10th birthday in Dublin in 2019 for isoscalars, exotics, ...
- Framework for scattering & coupled channels.

Terra Incognita

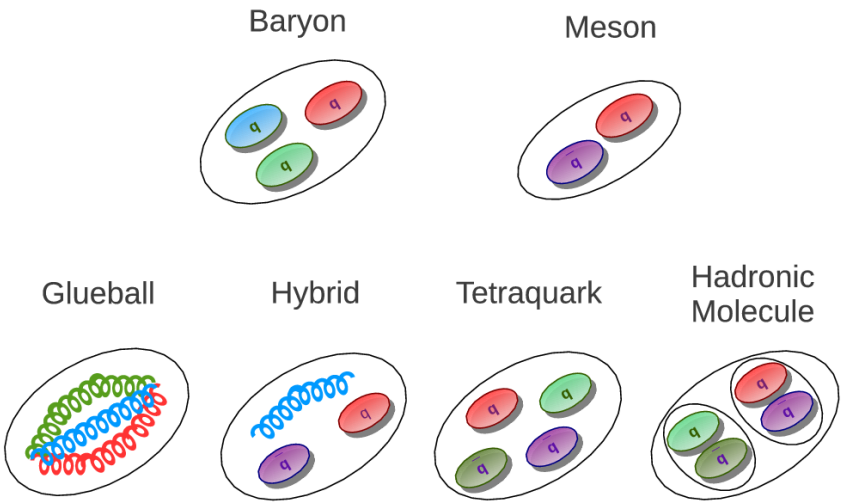
- Finite densit… …not valid!
- Scatte… …mperature ...

New ideas needed!

Open challenges

QCD spectroscopy

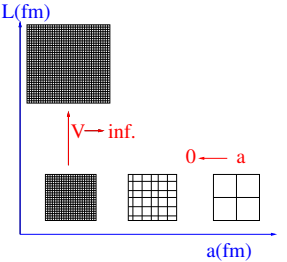
QCD admits a rich and exotic spectrum



[from M. Cleuven, 20140]

1. Working in a finite box at finite grid spacing

- Symanzik improvement at finite a.
- Recover continuum **QCD** by extrapolation.
  Costly but regular feature of precision lattice calculations.



2. Simulating at physical quark masses

- Computational and complexity costs of physical light and heavy quarks.
  Physical light quark simulations possible. Heavy quark systematics understood.

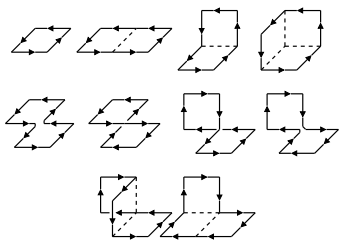
3. Breaking symmetry

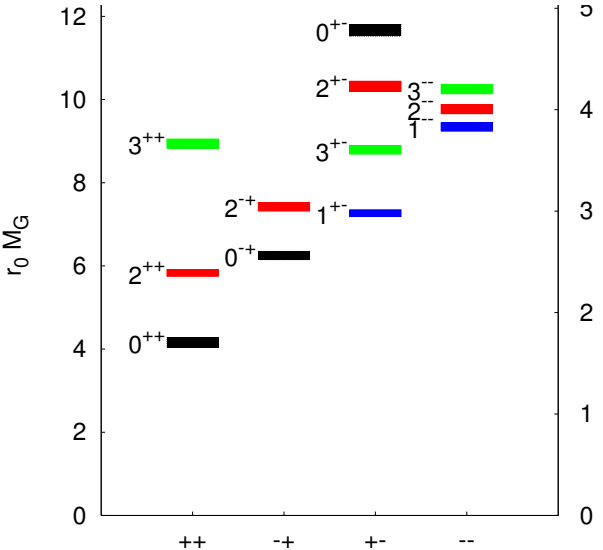
- Lorentz symmetry broken at $a \neq 0$: $SO(4)$ rotation group to rotation group of a hypercube. Define operators and identify states according to this symmetry.

4. Working in Euclidean time

- Gives access to energies via $C(t) \sim e^{-E_n t}$
- Scattering matrix elements not directly accessible from Euclidean QFT
  Lüscher formalism and generalisations allow indirect access - **exploiting the finite volume**.

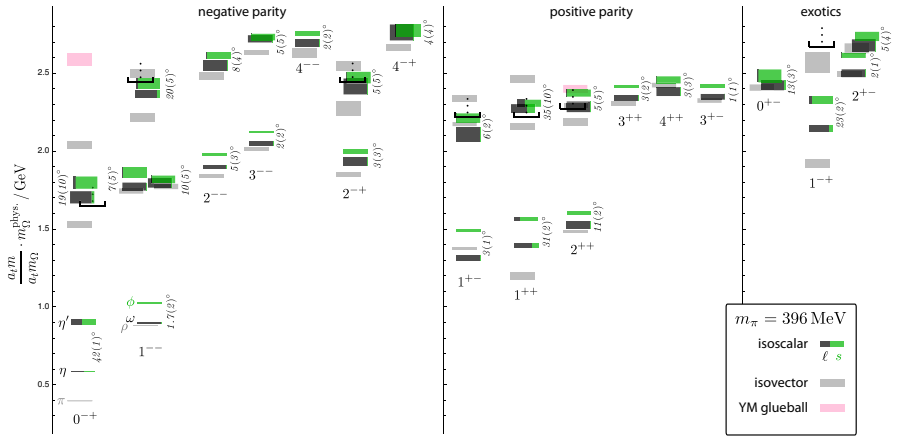
(Early) predictions: the glueball spectrum





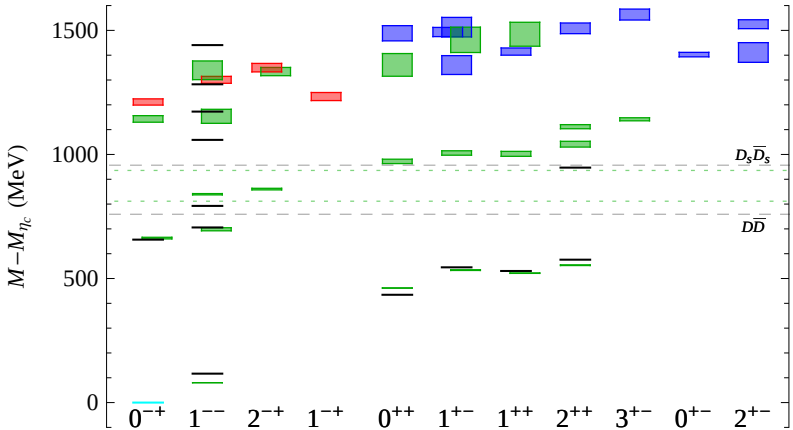
Morningstar & Peardon, 1999

Light mesons



from HSC 2012

Predictions: (exotic) hybrid meson in charmonium



- Spin exotic and non-exotic hybrids determined: enabled by *Distillation*
- Same pattern & energy scale in mesons and baryons, light and heavy.

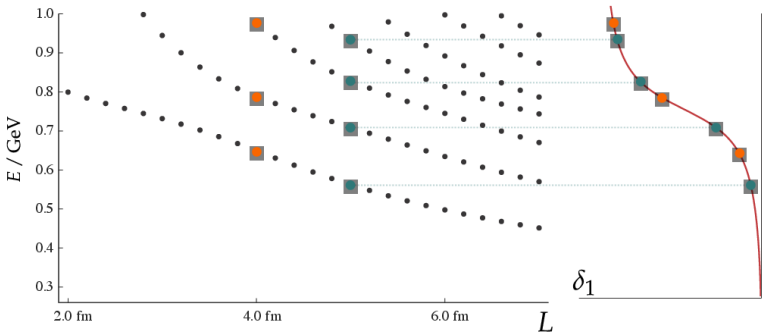
[Hadron Spectrum Collaboration, 2012]

Some Current Challenges in Lattice QCD

Beyond simple bound states: resonances in a Euclidean theory

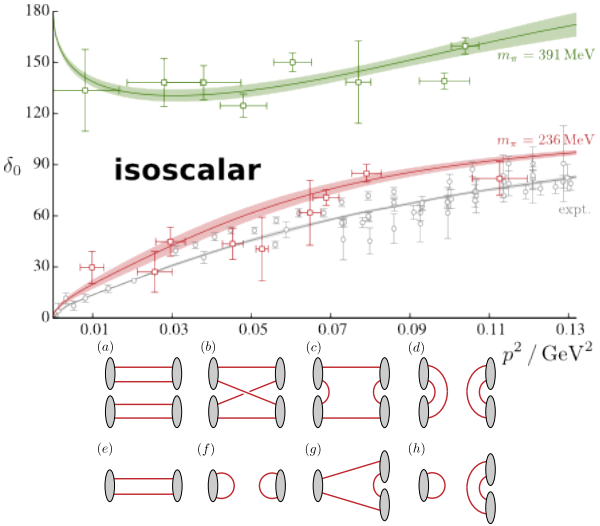
The problem: Lose direct access to scattering in a Euclidean QFT.
The solution: On lattice volumes extract the spectrum. Lüscher formalism (1991) allows to deduce phase shift information.

$$\det\left[\cot\delta(E_n^*) + \cot\phi(E_n, \vec{P}, L)\right] = 0$$



The more distinct spectrum points the better the phase shift picture

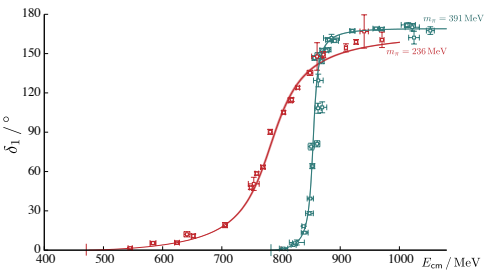
Recent examples in $\pi\pi$ scattering



σ evolves from bound-state below $\pi\pi$ threshold at heavier mass to broad resonance at lighter mass.

$$\det\left[\mathbf{1} + i\rho(E)\cdot\mathbf{t}(E)\cdot(\mathbf{1} + i\mathcal{M}(E,L))\right] = 0.$$

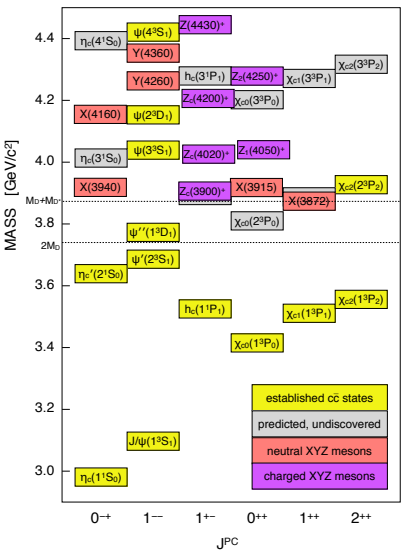
ρ resonance



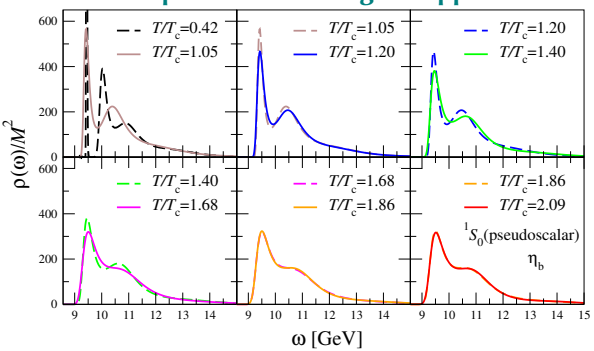
A tool to study mass-dependence!

Problems that we might solve ...

Strong Exotic Matter



Finite temperature: Melting & Suppression



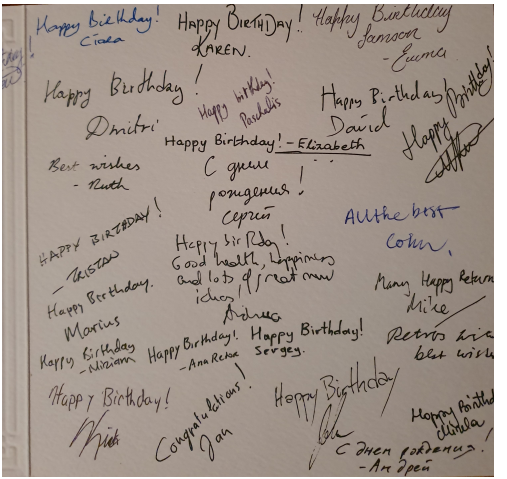
Perspectives

Classical computing

- Exascale computing within 5 years:
  - Not business as usual: significant mathematical algorithm development needed eg in numerical matrix inversion and determinant methods
  - Expect simulations with all uncertainties under control: physical quark masses, discretisation, volume.
  - Precision determinations of matrix elements relevant for SM and BSM phenomenology
  - New ideas for spectral reconstruction - currently limited as an ill-posed problem.
  - Exploiting ML/AI convergence with HPC for parameter scans, taming MEM ...
- Some old problems likely remain: for $\mu \neq 0$ - solving a sign problem

Quantum computing

- Sign problem, determinants?
- Some progress also on a “quantum” regularisation of the path integral
- A likely model is a quantum accelerator in a modular system.



Breithlá Shona duit a Shamson!!

go máire tú an lá