Heavy quark physics & lattice QCD: exploring strong matter

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Outline

- Setting the scene: particle physics
- QCD - a quantum theory for quarks and gluons
- Lattice QCD - calculating oberservable states to explore the phase diagram
- Selected recent results
- Summary & perspectives

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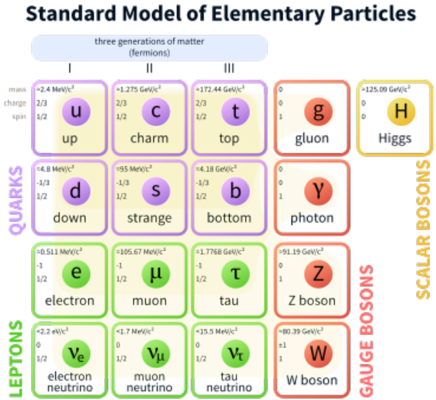
Many details and topics omitted for time constraints - APOLOGIES!

The particle physics landscape

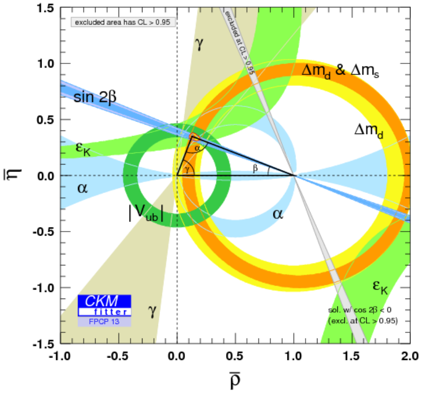


- Encompasses EM, strong & weak forces
- Embarassingly successful?
- Precision tests of SM may reveal new physics - more important than ever!
- Meanwhile, new strong exotic matter unexpectedly discovered
- Accurate & precise theoretical understanding of QCD is crucial.

Many unanswered questions remain:

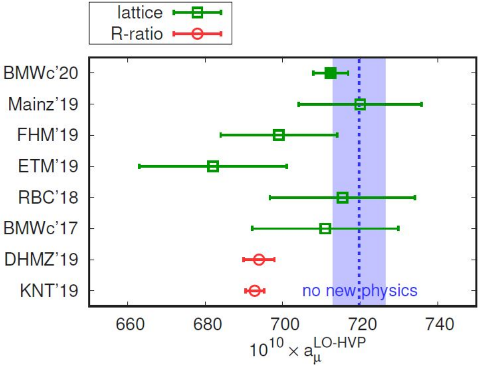
- What about gravity, dark matter, dark energy?
- How can we understand the matter-antimatter asymmetry?
- Are quarks and leptons truly fundamental and why are there exactly 3 generations?
- ...

(Lattice) QCD for Standard Model phenomenology



CKM Physics

Borsanyi et al [2002.12347]



Muon g-2

Quantum Chromodynamics (QCD)

- Quantum field theory of the strong interaction binding quarks and gluons forming hadrons.
- The only experimentally realised strongly-interacting quantum field theory - highlights many subtleties.
- A paradigm for strongly-interacting theories in BSM physics and elsewhere.
- Many puzzles and challenges remain in this well-studied arena.

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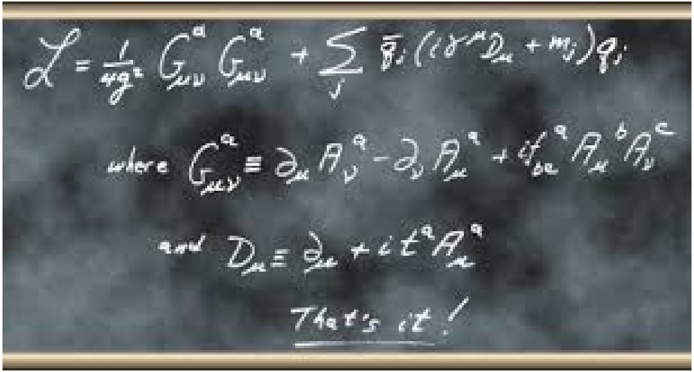


from F.A. Wilczek

QCD: a conceptually rich & practically powerful QFT

- Explains nature's strong interactions in terms of fundamental variables: quarks and gluons.
- A theory rich with symmetries!

$$SU(3)_C \times SU(3)_L \times SU(3)_R \times U(1)_A \times U(1)_B$$

  - Gauge "color" symmetry; Global chiral symmetry; Baryon number and axial charge (m=0) conservation. Scale invariance and discrete C, P, T symmetries.
- Gluons (force carriers) are charged under the strong interaction: very different to QED
- Quantum effects $\longrightarrow$ breaking of symmetries $\longrightarrow$ visible matter.
- Inherent properties of this relativistic field theory: confinement, asymptotic freedom, anomalies, SSB - depend on non-linear dynamics in QCD

Dynamical mass generation through non-linear interactions

Nothing to do with Higgs!

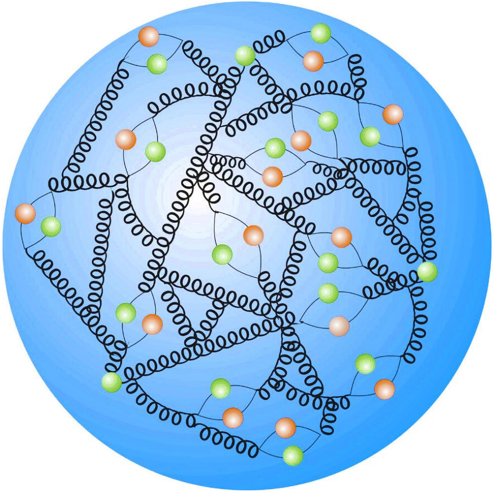
Massless gluons and almost massless quarks interact - generating most of the mass of nucleons

Proton: uud

- $m_u = 2.3^{+0.7}_{-0.5}$ MeV/c^2
- $m_d = 4.8^{+0.7}_{-0.3}$ MeV/c^2
- $m_P = 938.3$ MeV/c^2

- Only 1% of the proton's mass comes from the constituent quarks' intrinsic masses.
- The proton is an emergent (long-range) phenomena resulting from the collective behaviour of quarks and gluons - QCD.

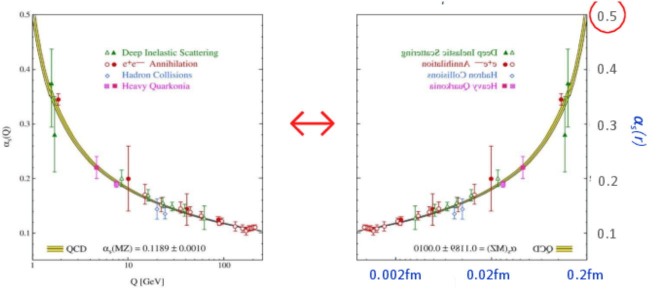
The secret life of protons



- A proton is composed of quarks, bound together by gluons
- QCD is the mathematical framework describing how these constituents interact.
- Confinement is purely quantum phenomenom and not yet understood

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**, $\Lambda_{QCD} \sim 300 MeV = \mathcal{O}(1 fm^{-1})$
- 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
  - conceptual and practical complications can make this challenging!
- Facilitates numerical simulation
  - MCMC approach drawing from methods in statistical physics systems
- 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.

Practicalities of a lattice calculation

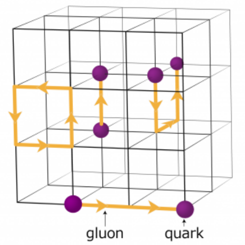
for spectroscopy

A lattice QCD primer

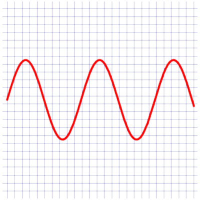
Start from the QCD Lagrangian:

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

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



Lattice acts as UV and IR regulator:



- typical spacing: $0.04\text{fm} \leq a \leq 0.2\text{fm}$ $(1\text{GeV} \leq a^{-1} \leq 5\text{Gev})$
- typical length: $2\text{fm} \leq L \leq 6\text{fm}$.
- (UV) $am_q \ll 1$; (IR) $M_\pi L \geq 4$

- Solve the QCD path integral on a finite lattice with spacing $a \neq 0$ with Monte Carlo in a Euclidean space-time metric (no useful importance sampling weight in Minkowski space).

  Observables determined from (Euclidean) path integrals of the QCD action

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

- In principle the finite temporal extent implies a finite temperature e.g

$$S_f[\bar{\psi},\psi,A_\mu] = \int_0^{1/T} d\tau \int_V d^3x \sum_f \bar{\psi}_f(x)\left(\gamma_\mu D_\mu + m_f\right)\psi_f(x)$$

- Change the temporal extent to change $T = 1/aN_t$

Correlators in Lattice Euclidean Field Theory

- 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 $(\Psi, \bar{\Psi}) \rightarrow$

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

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

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

- Correlation functions have a (improvable!) statistically uncertainty $\sim 1/\sqrt{N_{cfg}}$.
- $\det M$ swapped for M^{-1}, also required in correlation functions. Can take $> 80\%$ of compute cycles in configuration generation. $\det M = 1$: quenched approximation.

A recipe for (meson) spectroscopy

- Construct a basis of local and non-local operators $\bar{\Psi}(x)\Gamma D_i D_j \ldots \Psi(x)$ e.g. from *distilled* fields [Peardon, PRD80 (2009) 054506].
- Build a correlation matrix of two-point functions

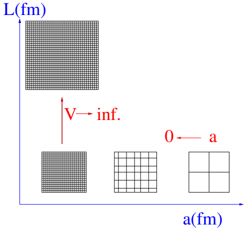
$$C_{ij} = \langle 0|\mathcal{O}_i \mathcal{O}_j^\dagger|0\rangle = \sum_n \frac{Z_i^n Z_j^{n\dagger}}{2E_n} e^{-E_n t}$$

- 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 $Z_i^{(n)} = \sqrt{2E_n} e^{E_n t_0/2} v_j^{(n)\dagger} C_{ji}(t_0)$

- Results shown here for anisotropic lattices $a_t \ll a_s$.

The compromises and consequences



1. Working in a finite box at finite grid spacing

- Recover continuum QCD by extrapolation.
  Part of the error budget.

2. Simulating at physical quark masses

- Computational and complexity cost of physical light and heavy quarks.
  Physical light & heavy quarks in reach. Mass dependence is a tool!

3. Breaking symmetry

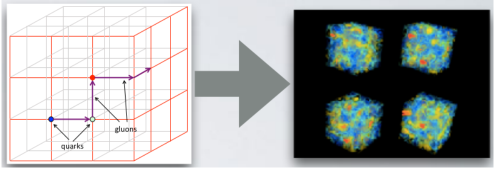
- Lorentz symmetry broken at $a \neq 0$: $SO(4)$ rotation group to rotation group of a hypercube.
  Identify states according to this symmetry.

4. Euclidean time

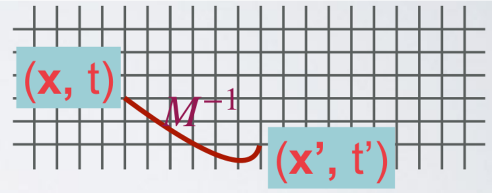
- Access energies via $C(t) \sim e^{-E_n t}$. Direct access to scattering matrix elements lost.
  Lüscher formalism and generalisations allow indirect access via finite volume.

Computing Lattice QCD

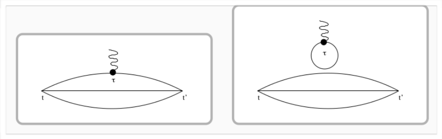
1. Ensemble generation
Markov Chain Monte Carlo → ensembles of gauge fields according to the QCD path integral. Stored/reused.



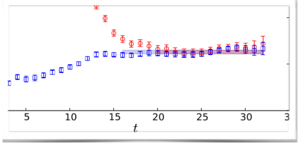
2. Quark Propagation
Solve $Mx = b$ for each spin, colour. M the Dirac matrix, b the source for quark propagator.



3. Contracting quark fields
Quark propagators contracted with operators to produce desired quantum numbers → correlation functions.

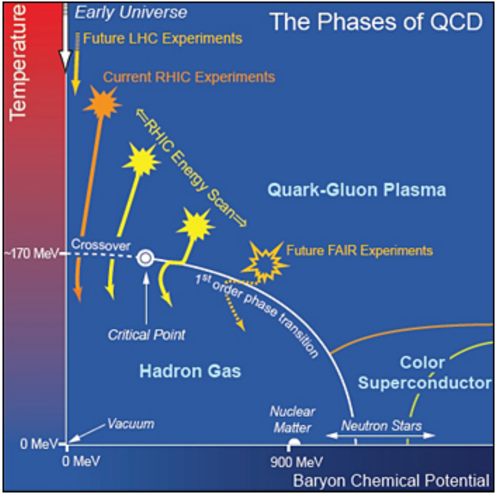


4. Data analysis
Physics (energies, form factors, etc) from correlation functions.



QCD & heavy quark phenomenology

The fate of strongly interacting matter



- Lattice QCD explores the temperature axis
  - EoS known in continuum limit, physical quark masses.
  - Hadron spectroscopy challenges: T>0 solving an inverse problem. T=0 extracting precision resonance parameters
  - Expensive: high statistics (many operators, temperatures needed).
- Finite density is fundamentally harder - no MC approach.

Quarkonia - bound states of heavy quarks

What is it?

- Flavourless mesons built from a heavy quark ($m_c \sim 1.3GeV$ or $m_b \sim 4.7GeV$) and its own antiquark: **Charmonium** ($c\bar{c}$) and **Bottomonium** ($b\bar{b}$). [No toponium due to the short lifetime of the top quark]

Some properties:

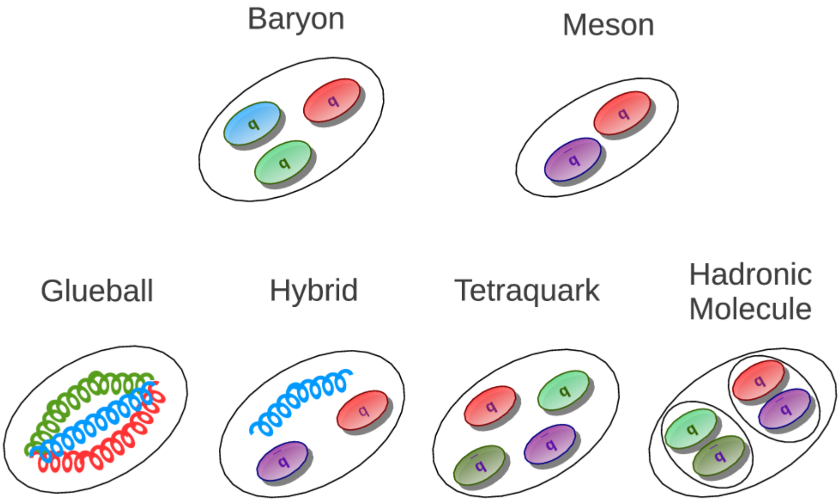
- Stable under strong decay while
  - Charmonium: $M_{c\bar{c}} < 2M_D \sim 2 * 1.9GeV$ for $D = c\bar{u}$
  - Bottomonium: $M_{b\bar{b}} < 2M_B \sim 2 * 5.3GeV$ for $B = b\bar{u}$

  Includes $\eta_c, J/\Psi, \Upsilon, \eta_b, \chi_{b0,b1,b2}$, ground state S and P waves.
- Many useful symmetries - e.g. spin and flavour.
- A fertile hunting ground for strong exotic matter.

Theoretical calculations:

- Potential models, sum rules, Lattice...
- Lattice methods now very precise - cf HadSpec Collaboration
- b-quarks well-suited to effective field theory methods on the lattice - HQET, NRQCD.

QCD admits a rich and exotic spectrum

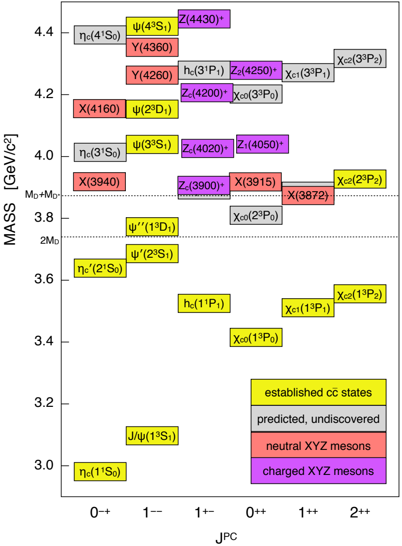


Includes J^{PC} not accommodated in quark models.

[from M. Cleuven, 20140]

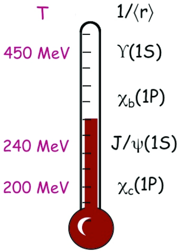
Experimental data: challenges in heavy quark spectroscopy

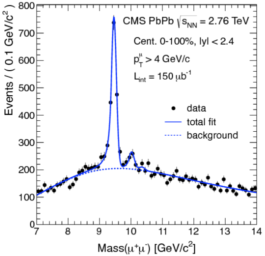
Zero temperature
understanding strong *exotic* matter

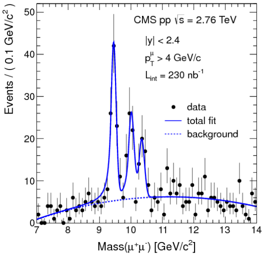


R.Mitchell & S. Olsen

Finite temperature
melting & suppression to probe the QGP







CMS (2012) PbPb [top] vs pp [bottom]

$T \sim 0$

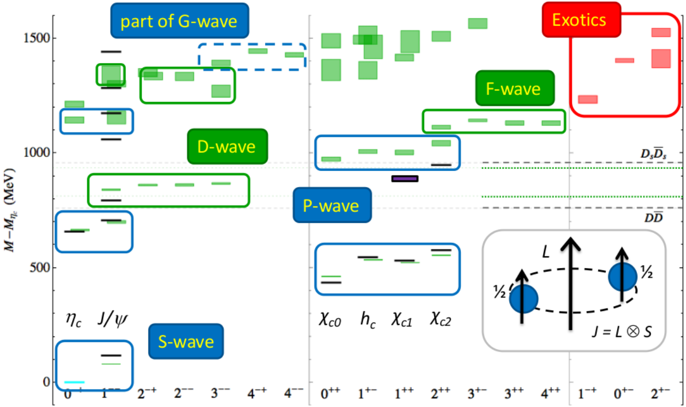
First step: understand the spectrum

Precision calculation of high spin ($J \geq 2$) and exotic charmonium states

Caveat Emptor

- Large basis of single-hadron (only) operators
- Physics of multi-hadron states appears to need relevant operators
- No continuum extrapolation
- Heavy pions (400 MeV). Also now with $m_\pi \sim 236$ MeV.

Charmonium

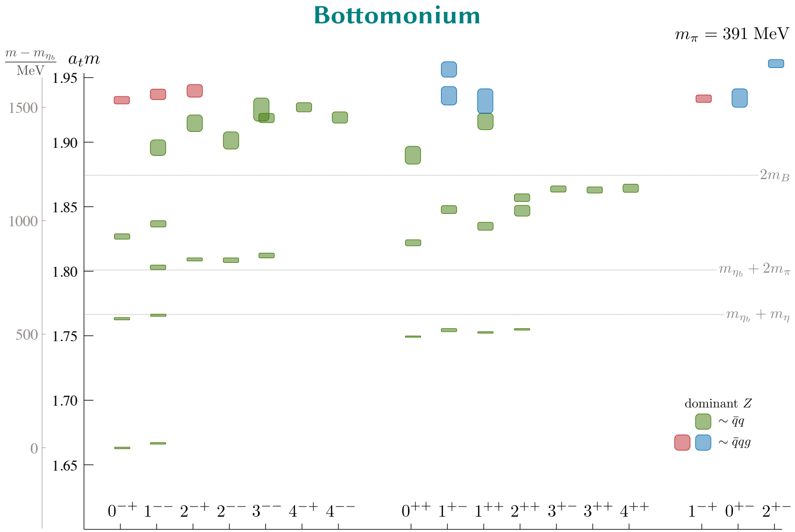


HSC 2012 [1204.5425]

XYZs are at/above (many) thresholds a huge challenge ...

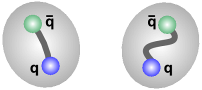
The same techniques applied to b quarks - an exploratory study

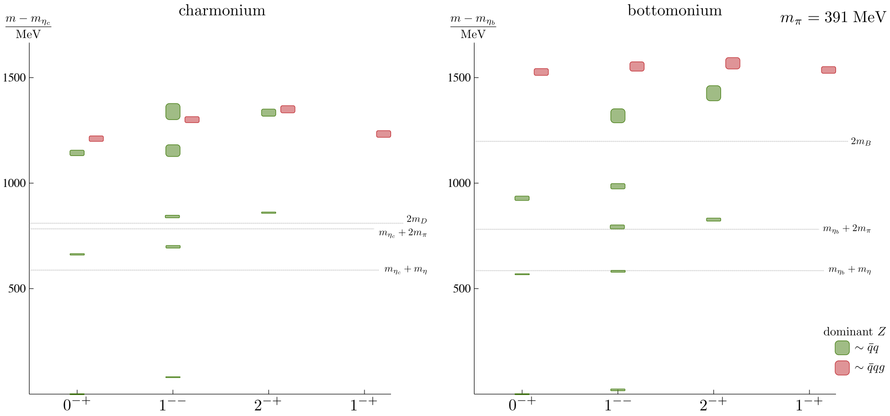
First determination of the excited and exotic bottomonium spectrum



from D. Wilson & SR, 2020 [2008.02656]

Hybrid Mesons (exotic & non-exotic)



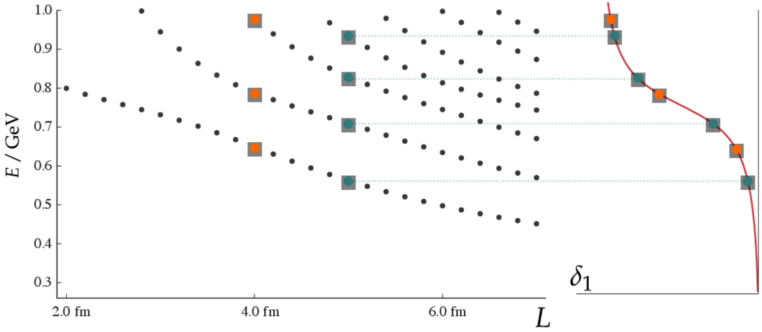


Lightest hybrid supermultiplets[*HadSpec*:2008.02656]: same pattern and scale also seen in open charm and light[*HadSpec*:1106.5515] sectors.

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.

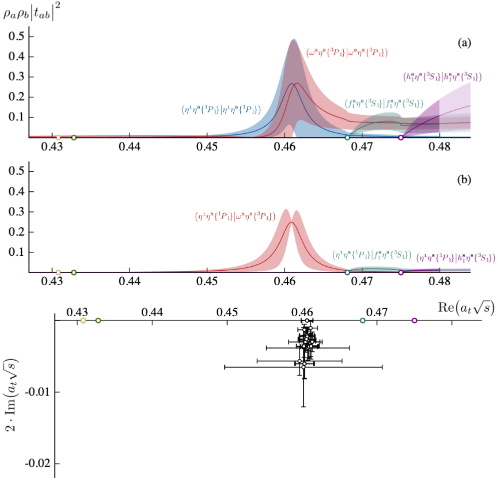
$$\det\left[\cot\delta(E_n^*) + \cot\phi(E_n,\vec{P},L)\right] = 0$$



The more distinct spectrum points the better the phase shift picture

Recent examples - scattering in exotic and non-exotic channels

A first look: light hybrid 1^{-+} resonance [2009.10034]



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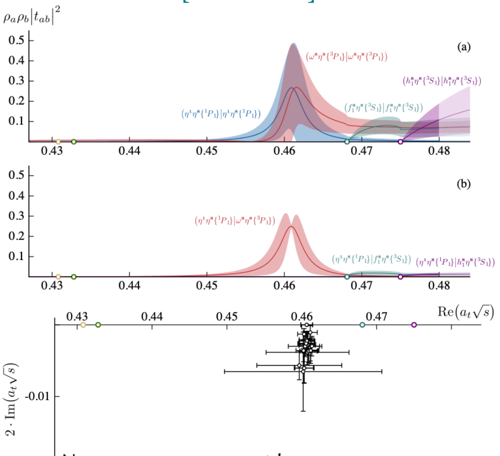
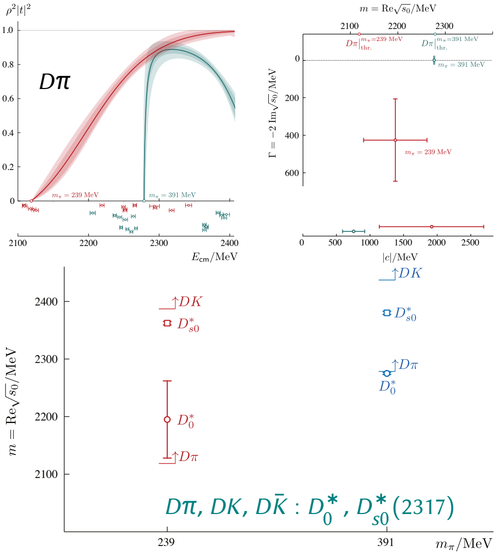


Narrow π_1 resonance at heavy m_π

Pole couplings suggest broad resonance at lighter m_π

Heavy-light meson scattering [2008.06432, 2102.04973]



$D\pi$, DK, $D\bar{K}$: D_0^* , $D_{s0}^*(2317)$

$T > 0$

Quarkonia at finite temperature

From correlation functions determine spectral functions: all information on thermal modifications of the spectrum in that channel.

$$C_i(\tau) = \int d\omega K(\tau,\omega)\rho_i(\omega) \quad \text{and} \quad K(\tau,\omega) = \frac{\cosh\left[\omega\left(\tau - \frac{1}{2T}\right)\right]}{\sinh\left(\omega/2T\right)}$$

ρ (a function of the continous energy) from (discrete) C: an ill-posed problem.

Maximum Entropy Method (a Bayesian approach) [See ECT* Workshop, Sept 2021]

- Construct ρ that maximises conditional probability $P[\rho|DH]$ of having ρ, given data D and prior H.
- Choice of prior (eg posititivty of ρ) defines the method - MEM based on Shannon Jaynes entropy, S:

$$P[\rho|DH] = exp(-\frac{1}{2}\chi^2 + \alpha S), \quad \text{with} \quad S = \int d\omega\left[\rho(\omega) - m(\omega) - \rho(\omega)\log\left(\frac{\rho(\omega)}{m(\omega)}\right)\right]$$

Quarkonia at finite temperature: MEM & NRQCD

- $\mathcal{L}_{\mathrm{nrqcd}}$ ordered in powers of $v = |\mathbf{p}|/m_Q$ and $v^2 \sim 0.1$ for b quarks.
- Propagators - solving an initial value problem

$$G(\mathbf{x}, \tau = 0) = S(\mathbf{x}) \; G(\mathbf{x}, \tau = a_\tau) = \left(1 - \frac{H_0}{2n}\right)^n U_4^\dagger(\mathbf{x}, 0) \left(1 - \frac{H_0}{2n}\right)^n G(\mathbf{x}, 0).$$

In NRQCD:

- No thermal boundary condition (kinematical temperature dependence) - a simple spectral relation: $G(\tau) = \int_{-2M}^{\infty} \frac{d\omega'}{2\pi} e^{-\omega'\tau} \rho(\omega'), \quad (\omega = 2M + \omega')$.
  Heavy quarks not in thermal equilibrium with light-quark-gluon system but appear as probes.

What to expect when quarks are not bound?

Consider free quarks in continuum NRQCD, with $E_{\mathbf{p}} = \frac{\mathbf{p}}{2M}$

As an example: S and P wave correlators

Burnier, Laine, Vepsäläinen '08

$$C_S(\tau) \sim \int d^3p \quad exp(-2E_{\mathbf{p}}\tau) \sim \tau^{-3/2}$$

$$\rho_S(\omega) \sim \int d^3p \quad \delta(\omega - 2E_{\mathbf{p}})$$

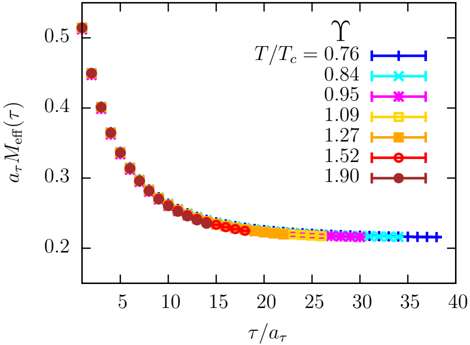
$$C_P(\tau) \sim \int d^3p \quad \mathbf{p}^2 exp(-2E_{\mathbf{p}}\tau) \sim \tau^{-5/2}$$

$$\rho_P(\omega) \sim \int d^3p \quad \mathbf{p}^2\delta(\omega - 2E_{\mathbf{p}})$$

- Temperature dependence only enters via the medium!
- In the free continuum case - power law decay for large euclidean time, τ
- Expect modifications from interactions, finite lattice spacing, etc in a realistic case

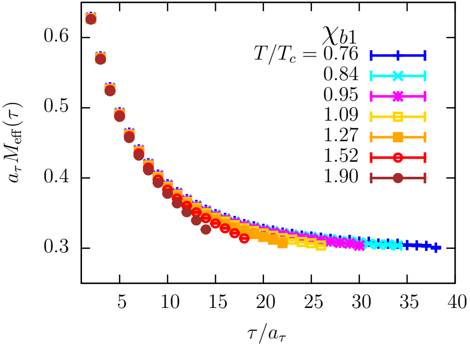
Effective Mass: comparing S and P wave correlators

Υ : S wave



Very little T dependence.

χ_{b1} : P wave

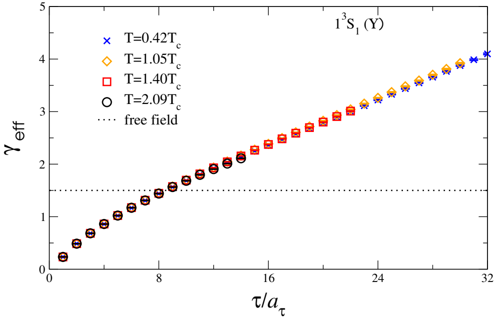


Significant T dependence. Rules out pure exponential decay at $T \sim 2T_c$

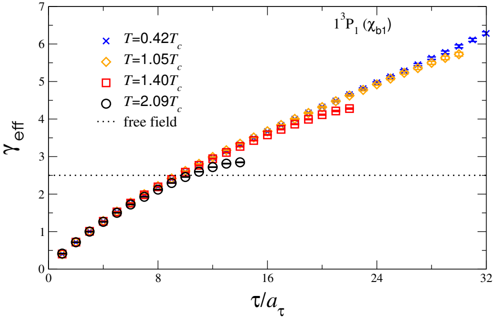
[these and following from 1402.6210 and 1912.09827]

Effective power: Comparing S and P wave correlators

$$\gamma_{\text{eff}} = -\tau \frac{G'(\tau)}{G(\tau)} \to \tau$$



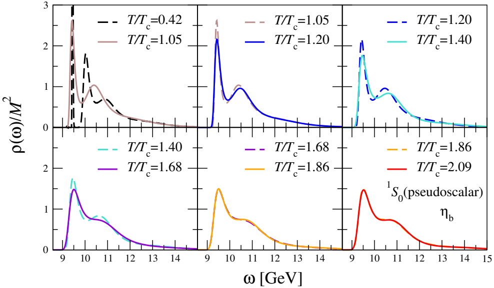
Υ S wave



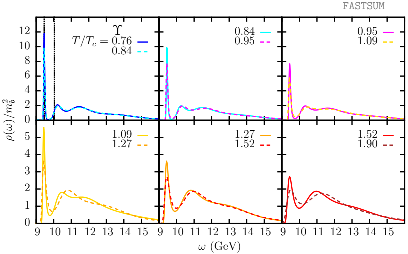
χ_{b1} P wave

S waves in detail with MEM: Υ and η_b in the plasma

η_b : S wave

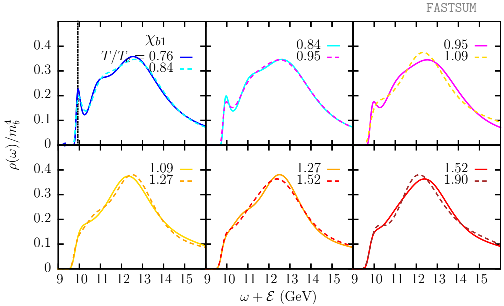


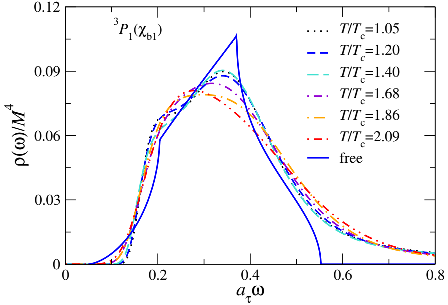
Υ : S wave



- η_b ground state survives - excited states suppressed
- Υ ground state survives - excited states suppressed.
- Similar results from CMS.

P waves in detail from MEM: χ_{b1} in the plasma





- Other χ_b states similar.
- Structure of spectral functions from NRQCD similar to $\rho^{\text{free,lat}}_{\text{Pwave}}(\omega)$.
- Clear indications of melting immediately above T_c and of unbound, quasi-free b quarks.

Summary & Outlook

- A renaissance in lattice heavy quark spectroscopy - mapping the spectrum of excited and exotic states, tackling resonances (only briefly discussed) and probing the QGP.
- Full scattering "machinery" honed in light sector, now to be applied for XYZs.
- EFTs (e.g. NRQCD) can play a crucial role, including at finite T.
- Full error budgets for resonances and for T>0 still to come.
- Many open questions and little dialogue to date between the T=0 and T>0 communities, lots of interesting avenues ...
  - Distillation & variational analysis at finite temperature for unstable states, transport?
  - Melting and suppression may yield information on structure of exotic states?

Many challenges remain ...

Perspectives

Classical computing

- Exascale computing within 5 years:
    - Not business as usual: significant algorithm development needed eg in numerical matrix inversion and determinant methods.
    - Look forward to simulations with all(?) uncertainties under control: physical quark masses, discretisation, volume.
    - A new era for precision determinations of SM and BSM phenomenology
    - Exploiting ML/DL convergence with HPC for parameter scans & tuning, taming inverse problems ...
- Some old problems likely remain: for $\mu \neq 0$ - solving a sign problem

Quantum computing

- Sign problem, determinants?
- Is a likely model a quantum accelerator in a modular system. How can we exploit this?

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Many challenges remain ...  *... Thanks for listening!*