

Lattice simulations for charm

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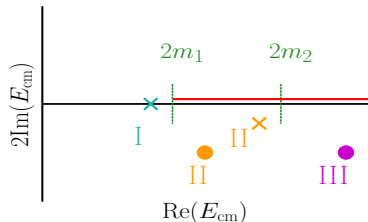
18th January, 2024

FTCF 2024 - USTC Hefei China

:ONLINE:

- ❁ Spectroscopy of hadrons involving charm quarks:
 - Strong interaction stable hadrons,
Baryons and mesons,
Shallow bound states and unstable resonances.
Tetraquarks, pentaquarks, hexaquarks, etc.
My talk will focus on this.
Although I do not intend for an extensive review.

- ❁ Flavor physics, heavy quark masses, etc.
 - Will not be covered.

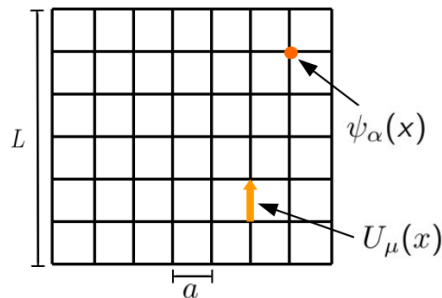


<http://flag.unibe.ch/2021/>

Lattice QCD: Basic idea

LQCD : A non-perturbative, gauge invariant regulator for the **QCD** path integrals.

- ✿ Quark fields $\psi_\alpha(x)$ on lattice sites
- ✿ Gauge fields as parallel transporters U_μ
Lives in the links. $U_\mu(x) = e^{igaA_\mu(x)}$
- ✿ $\bar{\psi}_\alpha^i(x)[U_\mu(x)]_{ij}\psi_\alpha^j(x + a\hat{\mu})$ is gauge invariant.
- ✿ Lattice spacing : UV cut off
- ✿ Lattice size : IR cut off



Employ Monte Carlo importance sampling methods on Euclidean metric for numerical studies.

QCD spectrum from Lattice QCD

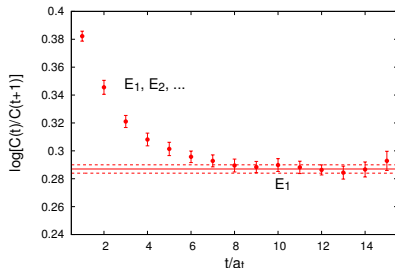
- ❁ Aim : to extract the physical states of QCD.
- ❁ Euclidean two point current-current correlation functions

$$C_{ji}(t_f - t_i) = \langle 0 | \mathcal{O}_j(t_f) \bar{\mathcal{O}}_i(t_i) | 0 \rangle = \sum_n \frac{Z_i^{n*} Z_j^n}{2m_n} e^{-m_n(t_f - t_i)}$$

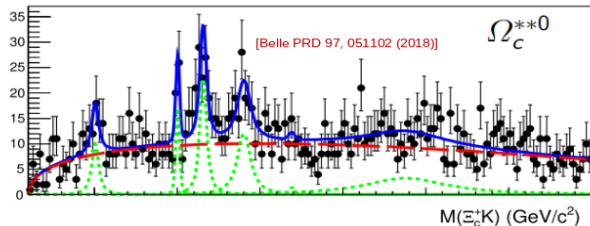
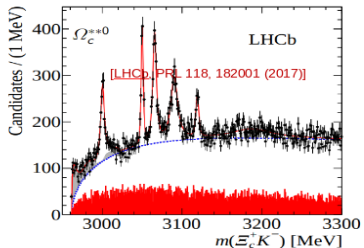
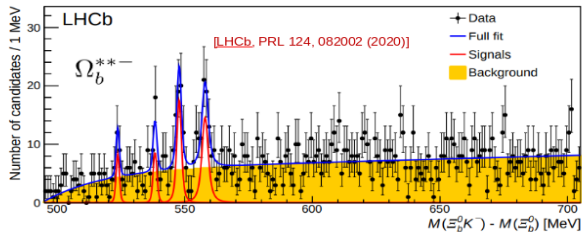
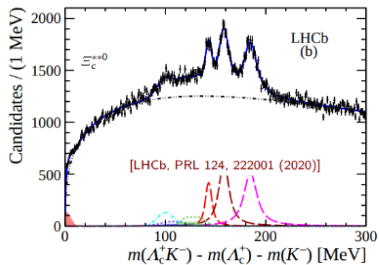
where $\mathcal{O}_j(t_f)$ and $\bar{\mathcal{O}}_i(t_i)$ are the desired interpolating operators and $Z_j^n = \langle 0 | \mathcal{O}_j | n \rangle$.

- ❁ Effective mass defined as $\log\left[\frac{C(t)}{C(t+1)}\right]$

- ❁ The ground state : from the exponential fall off at large times.
Non-linear fitting techniques.

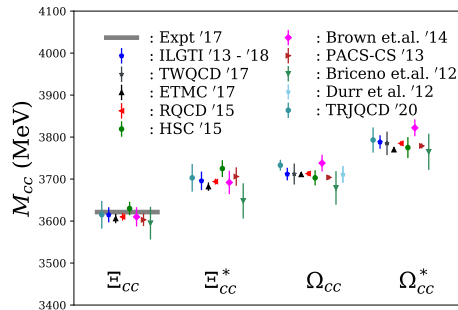
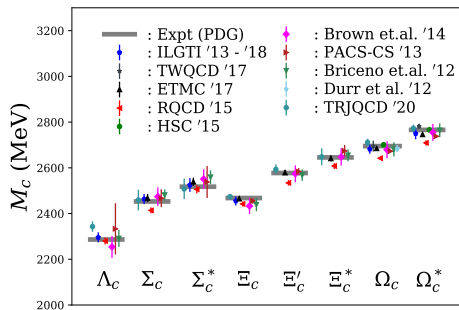


Heavy baryons in experiments



More in the talks by Liming Zhang and Xiang Liu

Singly and doubly charm baryons



Padmanath Lattice 2018

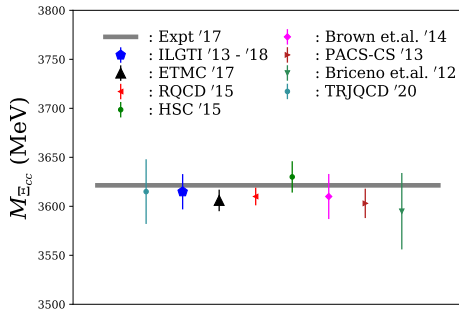
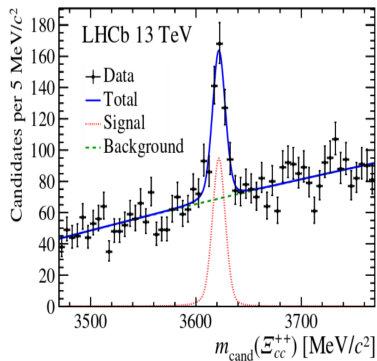
Another calculation of heavy baryon masses: QCDSF-UKQCD 1711.02485.

Heavy baryon mass splittings : BMW Science347 1452 '15

Early quenched lattice calculations : Lewis et al. '01; Mathur et al. '02; Flynn et al. '03

Dynamical (light quark) investigations : Liu et al. '10

The first doubly charm baryon : Ξ_{cc}



Ξ_{cc} isospin splitting (LQCD), 2.16(11)(17) MeV : BMW Science347 1452 '15

SELEX measurement (3519 MeV) : Mattson *et al.* PRL89 112001 '02

All lattice calculations disfavours SELEX peak to be a doubly charm baryon.

More on heavy baryon interactions [in this link](#).

Excited heavy baryon spectrum

✿ Recent discoveries: Ω_c^{**0} , $\Omega_b^{** -}$, and Ξ_c^{**0} .

✿ Challenges include extracting densely populated spectra.

Extracting densely populated states

Extracting radial and orbital excitations

Extracting excitations with spin $> 3/2$

Systematic spin identification

Multiple scattering channels affecting the single hadron spectra

✿ Scattering parameters from finite volume energy shifts.

Lüscher's formalism and its generalizations.

Lüscher 1991, Briceño 2014 and references and references therein

✿ Encouraging achievements in the light and heavy meson spectra.

c.f. yearly Lattice conference proceedings

The variational method

Two-point correlator

$$C_{ij}(t) = \langle 0 | \Phi_i(t) \Phi_j^\dagger(0) | 0 \rangle$$

$$C_{ij}(t) = \sum_{\mathbf{n}} e^{-E_{\mathbf{n}} t} \langle 0 | \Phi_i(0) | \mathbf{n} \rangle \langle \mathbf{n} | \Phi_j^\dagger(0) | 0 \rangle$$

$$Z_i^{\mathbf{n}} \equiv \langle \mathbf{n} | \Phi_i^\dagger | 0 \rangle$$

Matrix of correlators

$$C(t) = \begin{pmatrix} \langle 0 | \Phi_1(t) \Phi_1^\dagger(0) | 0 \rangle & \langle 0 | \Phi_1(t) \Phi_2^\dagger(0) | 0 \rangle & \cdots \\ \langle 0 | \Phi_2(t) \Phi_1^\dagger(0) | 0 \rangle & \langle 0 | \Phi_2(t) \Phi_2^\dagger(0) | 0 \rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

“Rayleigh-Ritz method”

Diagonalize:

eigenvalues \rightarrow spectrum

eigenvectors \rightarrow spectral “overlaps” $Z_i^{\mathbf{n}}$

Each state optimal combination of Φ_i

$$\Omega^{(\mathbf{n})} = \sum_i v_i^{(\mathbf{n})} \Phi_i$$

Benefit: orthogonality for near degenerate states

Baryon operators

Construction : permutations of 3 objects

- **Symmetric:**
 - e.g., uud+udu+duu
- **Antisymmetric:**
 - e.g., uud-udu+duu-...
- **Mixed:** (antisymmetric & symmetric)
 - e.g., udu - duu & 2duu - udu - uud

Multiplication rules:

- Symmetric Antisymmetric \rightarrow Antisymmetric
- Mixed \times Mixed \rightarrow Symmetric \oplus Antisymmetric \oplus Mixed
-

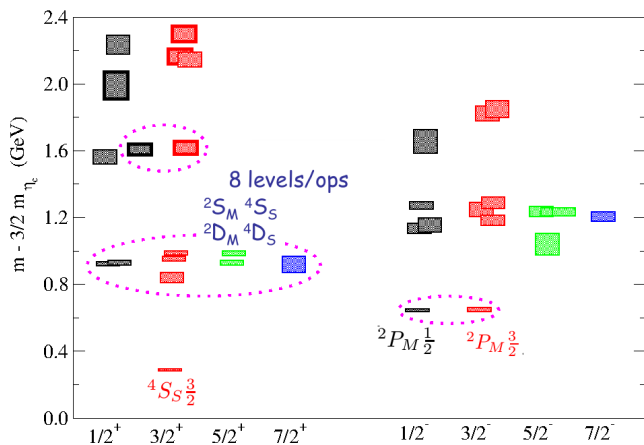
Color antisymmetric \rightarrow Require **Space \times [Flavor \times Spin]** symmetric

Space: couple covariant derivatives onto single-site spinors - build any J,M

$$\Phi^{JM} \leftarrow (CGC's)_{i,j,k} [\vec{D}]_i [\vec{D}]_j [\Psi]_k$$
$$J \leftarrow \mathbf{1} \otimes \mathbf{1} \otimes \mathbf{S}$$

Classify operators by permutation symmetries:

- **Leads to rich structure**

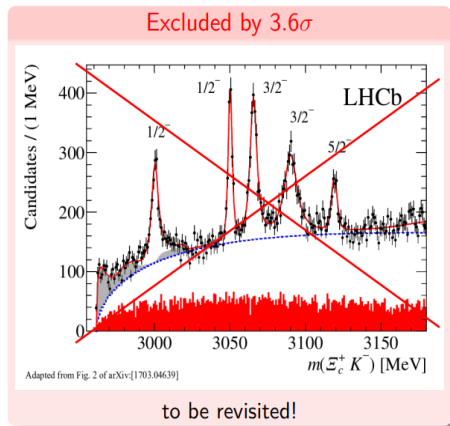
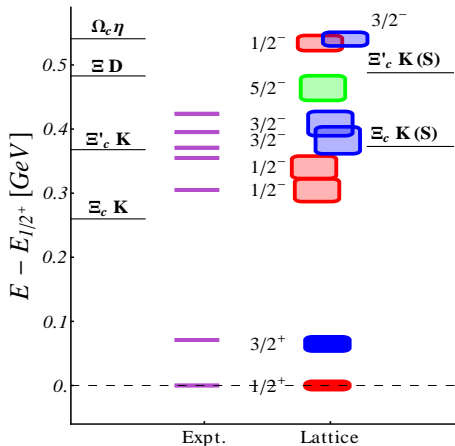
MP *et al* (HSC) 2013

Consistent with $SU(3)_F \otimes SU(2)_S \otimes O(3)$ expectations

Equivalent calculations of light baryons, Singly charm baryons, doubly charm baryons and triply bottom baryons.

See [this link](#).

Ω_c baryon: Quantum number assignment and falsification



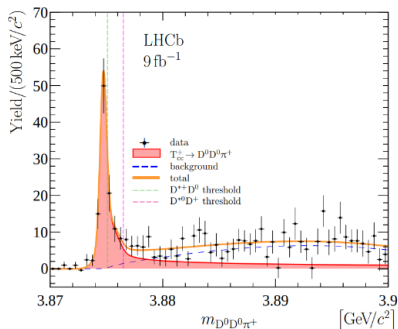
MP and Mathur 2017 PRL and other pheno predictions.

LHCb PRD 104, L091102 (2021)

Excited state studies achievements and caveats

- ✿ Systematic extraction of various radial and orbital excitations.
- ✿ Systematic methodology for spin identification.
- ✿ Broadly consistent with nonrelativistic quark model.
- ✿ No “freezing degrees of freedom”; no parity doubling.
- ✿ Yes! There are caveats
 - Relatively low statistics and no continuum limit.
 - Finite size effects; only one volume, $L \sim 2\text{fm}$
 - Heavy pion mass; $m_\pi \sim 400\text{MeV}$
 - only single hadron operators \Rightarrow No scattering/multihadron operators
- ✿ Outlook : Study the effects of baryon-meson interpolators, investigate widths.
Cost of computing increases.
- ✿ More experimental results can motivate lattice practitioners to take up these challenges.
Super tau Charm Factories could play a crucial role here.

Doubly heavy tetraquarks: T_{cc}^+



LHCb: 2109.01038, 2109.01056

$$\delta m \equiv m_{T_{cc}^+} - (m_{D^{*+}} + m_{D^0})$$

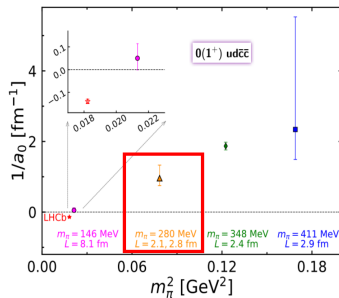
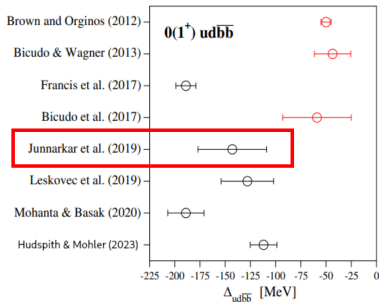
$$\delta m_{\text{pole}} = -360 \pm 40_{-0}^{+4} \text{ keV}/c^2,$$

$$\Gamma_{\text{pole}} = 48 \pm 2_{-14}^{+0} \text{ keV}.$$

- ✿ The doubly charmed tetraquark T_{cc}^+ , $I = 0$ and favours $J^P = 1^+$. *Nature Phys.*, *Nature Comm.* 2022 Striking similarities with the longest known heavy exotic, X(3872).
- ✿ No features observed in $D^0 D^+ \pi^+$: possibly not $I = 1$.
- ✿ Many more exotic tetraquark candidates discovered recently, T_{cs} , $T_{c\bar{s}}$, X(6900). Prospects also for T_{bc} in the near future. *See talk by Ivan Polyakov at Hadron 2023*
- ✿ Doubly heavy tetraquarks: theory proposals date back to 1980s.

c.f. Ader&Richard PRD25(1982)2370

Motivation from lattice, T_{bb} and T_{cc}



✿ Isoscalar axialvector channel $I(J^P) = 0(1^+)$.

✿ Deeper binding in doubly bottom tetraquarks $\mathcal{O}(100\text{MeV})$.

Fig: Hudspith&Mohler 2023

Red box: Our previous work on QQ tetraquarks: Junnarkar et al. PRD 2019

✿ Shallow bound state in doubly charm tetraquarks $\mathcal{O}(100\text{keV})$.

Fig: HALQCD 2023

Red box: T_{cc} and its quark mass dependence, an upcoming work: stay tuned.

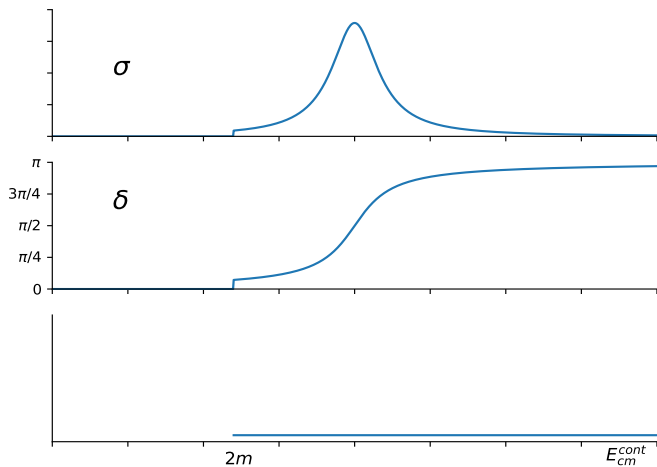
✿ No conclusive results in the bottom-charm tetraquark sector.

A summary of different lattice investigations \rightarrow

see review by Pedro Bicudo, 2212.07793

The challenge on lattice: Resonances in the infinite volume continuum

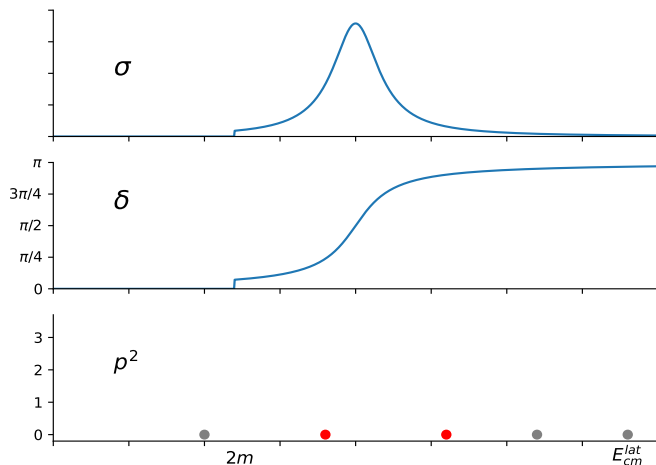
Scattering cross sections, phase shifts, branch cuts, Riemann sheets.



Schematic picture for illustration. Should not be taken quantitatively.

Resonances on the lattice (elastic) : ??

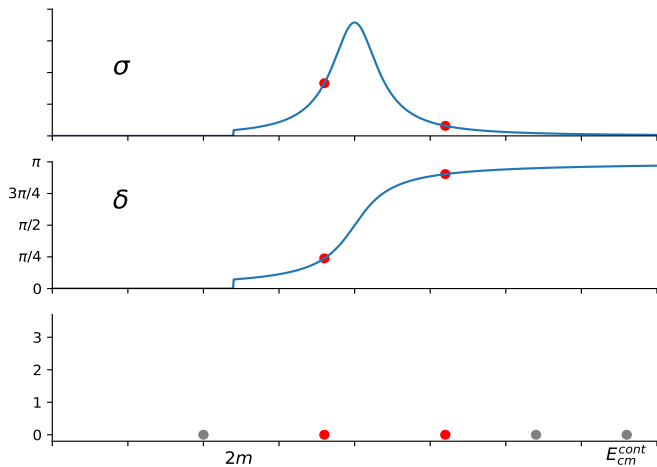
Discrete spectrum: No branch cuts, no Riemann sheets, no resonances!



Maiani-Testa no-go theorem [1990]

Resonances on the lattice (elastic) : Lüscher (1991)

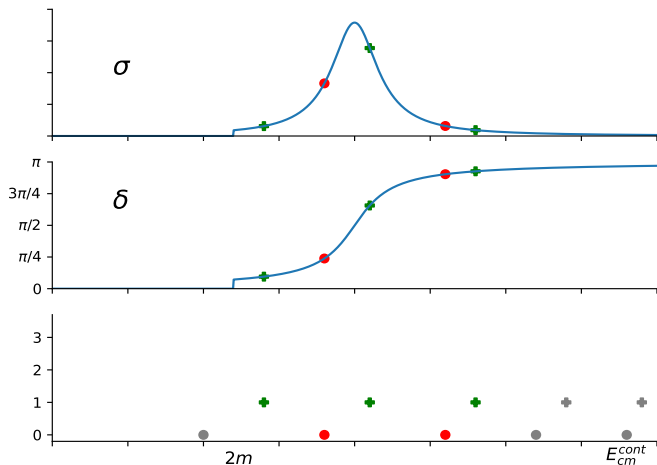
Infinite volume scattering amplitudes \Leftrightarrow Finite volume spectrum



Lüscher [1991]

Resonances on the lattice (elastic) : Lüscher (1991)

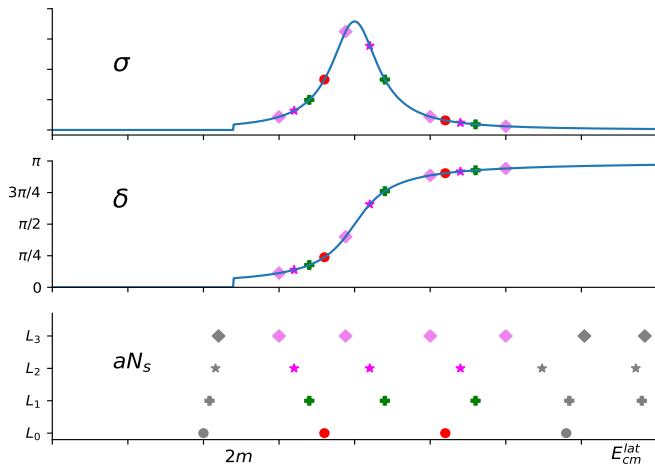
Infinite volume scattering amplitudes \Leftrightarrow Finite volume spectrum



Different inertial frames can be utilized to extract more information

Resonances on the lattice (elastic) : Lüscher (1991)

Infinite volume scattering amplitudes \Leftrightarrow Finite volume spectrum



Multiple physical volumes can also be utilized to extract more information.

For generalizations of Lüscher framework, *c.f.* Briceño, Hansen 2014-15

Finite volume spectrum and infinite volume physics

- On a finite volume Euclidean lattice : Discrete energy spectrum
Cannot constrain infinite volume scattering amplitude away from threshold.

Maiani-Testa 1990

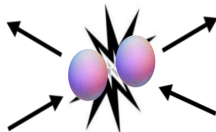
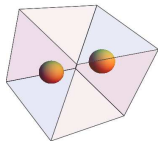
- Non-interacting two-hadron levels are given by

$$E(L) = \sqrt{m_1^2 + \vec{k}_1^2} + \sqrt{m_2^2 + \vec{k}_2^2} \text{ where } \vec{k}_{1,2} = \frac{2\pi}{L}(n_x, n_y, n_z).$$

- Switching on the interaction: $\vec{k}_{1,2} \neq \frac{2\pi}{L}(n_x, n_y, n_z)$. e.g. in 1D $\vec{k}_{1,2} = \frac{2\pi}{L}n + \frac{2}{L}\delta(k)$.

- Lüscher's formula relates finite volume level shifts \Leftrightarrow infinite volume phase shifts.

Lüscher 1991



- Generalizations of Lüscher's formalism: *c.f.* Briceño 2014
Quite complex problem: inelastic resonances ($R \rightarrow H_1 H_2, H_3 H_4$)

Scattering amplitude parametrization

❁ Scattering amplitude: $S = 1 + i \frac{4k}{E_{cm}} t$

❁ For an elastic scattering, and assuming only S -wave,

$$t^{-1} = \frac{2\tilde{K}^{-1}}{E_{cm}} - i \frac{2k}{E_{cm}}, \quad \text{with} \quad \tilde{K}^{-1} = k \cdot \cot \delta(k)$$

(virtual/bound) state constraint below threshold: $k \cdot \cot \delta(k) = (+/-) \sqrt{-k^2}$

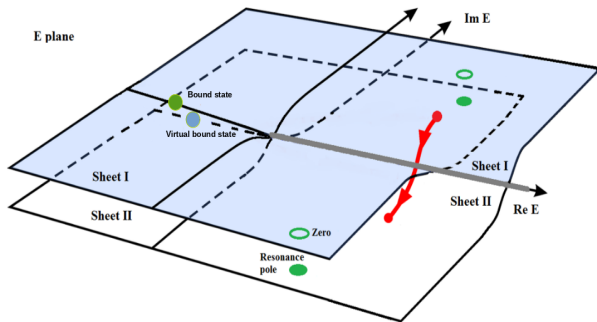
❁ Lüscher's prescription: $k \cdot \cot \delta(k) = \mathcal{F}(k)$, where $\mathcal{F}(k^2)$ is a known mathematical function. k^2 is determined from each extracted finite volume energy splittings.

❁ Parametrize $k \cdot \cot \delta(k)$ as different functions of k .

Effective Range Expansion (ERE): $k \cdot \cot \delta(k) = a_0^{-1} + 0.5r_0k^2 + \beta_i k^{2i+4}$.

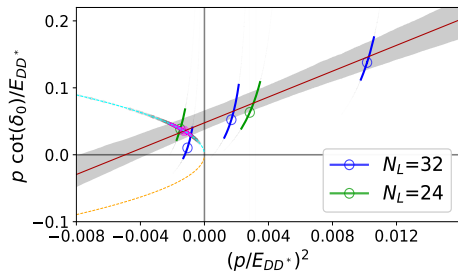
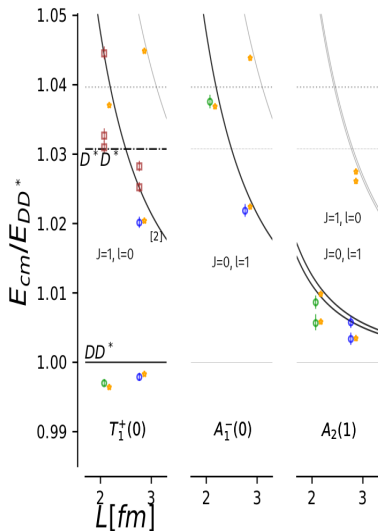
The best fits and fit estimates determined to represent the energy dependence of the amplitude.

Virtual/bound states



- ✿ $T \propto (pcot\delta_0 - ip)^{-1}$. Bound state is a pole in T with $p = i|p|$.
Virtual bound state is a pole in T with $p = -i|p|$.
- ✿ An example for virtual bound state: spin-singlet dineutron.

DD^* scattering in $l = 0, 1$ @ $m_c^{(h)}$ with an ERE



Fit quality:

$$\chi^2/d.o.f. = 3.7/5.$$

$m_\pi \sim 280$ MeV

Fit parameters:

$$a_0^{(1)} = 1.04(0.29) \text{ fm} \ \& \ r_0^{(1)} = 0.96_{(-0.20)}^{(+0.18)} \text{ fm}$$

$$a_1^{(0)} = 0.076_{(-0.009)}^{(+0.008)} \text{ fm}^3 \ \& \ r_1^{(0)} = 6.9(2.1) \text{ fm}^{-1}$$

Binding energy:

$$\delta m_{T_{cc}} = -9.9_{(-7.2)}^{(+3.6)} \text{ MeV}.$$

First evaluation of the DD^* amplitude in T_{cc} channel.

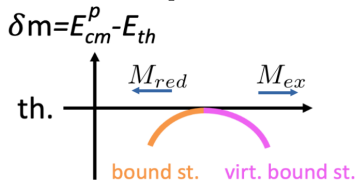
+g refers to positive parity, -/u refers to negative parity.

Our observations and inferences with ERE approach

- ✿ A shallow virtual bound state pole in s -wave related to T_{cc} .

	m_D [MeV]	$\delta m_{T_{cc}}$ [MeV]	T_{cc}
lat. ($m_\pi \simeq 280$ MeV, $m_c^{(h)}$)	1927(1)	$-9.9^{+3.6}_{-7.2}$	virtual bound st.
lat. ($m_\pi \simeq 280$ MeV, $m_c^{(l)}$)	1762(1)	$-15.0^{(+4.6)}_{(-9.3)}$	virtual bound st.
exp.	1864.85(5)	$-0.36(4)$	bound st.

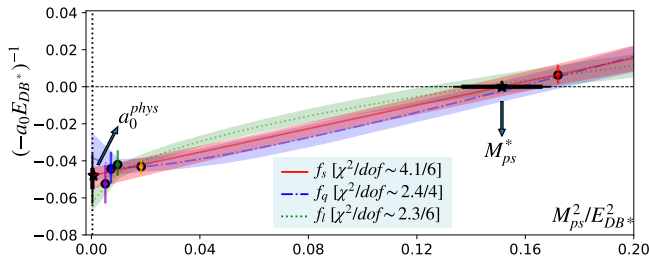
- ✿ For $m_\pi > m_\pi^{phys}$, T_{cc} is expected to become a virtual bound state. At $m_\pi \sim 280$ MeV, we indeed find a shallow virtual bound state.
- ✿ Observations in line with the expected behaviour of a near-threshold molecular bound state pole in simple Quantum Mechanical potentials.



See a recent talk by Sasa Prelovsek [here](#)

- ✿ $M_{red}(\propto m_c)$ is the reduced mass of the DD^* system.
- ✿ The mass of the particle exchanged during the interaction $M_{ex}(\propto m_{u/d})$.

$T_{bc} (I)J^P = (0)1^+$ bound state



MP *et al* 2307.14128, See a recent dedicated talk on this [here](#)

- Light quark mass ($m_{u/d}$ or M_{ps}) dependence indicates a real bound state at physical pion mass.
- DB^* scattering length¹ and binding energy (w.r.t. E_{DB^*}) in the continuum limit

$$a_0^{phys} = 0.57_{(-5)}^{(+4)}(17) \text{ fm} \quad \text{and} \quad \delta m_{T_{bc}} = -43_{(-7)}^{(+6)}_{(-24)}^{(+14)} \text{ MeV}$$

- A more recent lattice investigation also suggesting attractive interactions.

Alexandrou *et al* 2312.02925

¹Note the sign convention used: $[k \cot \delta_0 \sim -1/a_0]$

Pion exchange cuts/left-hand cuts and shortcomings with an ERE and QC

- ✿ A two fold problem: (Unphysical pion masses used in lattice)
 - ERE convergences fails at the left-hand cut.
 - $2 \rightarrow 2$ Generalized LQC does not incorporate such lhs effects.

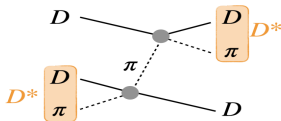
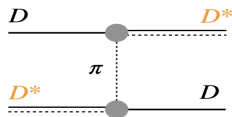


Figure taken from arXiv:2401.06609

- ✿ Unphysical pion masses ($m_\pi > \Delta M = M_{D^*} - M_D$, stable D^* meson):

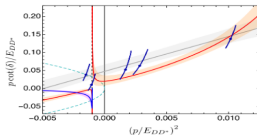
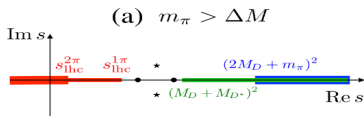
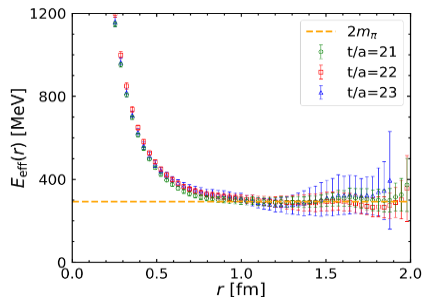


Figure taken from Meng-Lin Du *et al* arXiv:2303.09441[PRL]

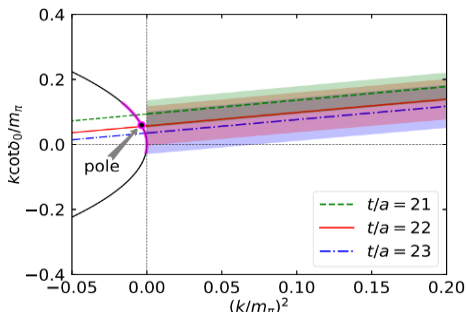
Fits with a potential that incorporates the one pion exchange:
 Virtual bound states \Rightarrow Virtual resonances

Alternatively: HALQCD approach @ near physical m_π

✿ DD^* s -wave scattering amplitudes from the lattice extracted DD^* potential.



$$E_{\text{eff}}(r) = -\frac{\ln[V(r)r^2/a_3]}{r}$$



$$V_{\text{fit}}^B(r; m_\pi) = \sum_{i=1,2} a_i e^{-(r/b_i)^2} + a_3 \left(1 - e^{-(r/b_3)^2}\right)^n V_\pi^n(r)$$

Lyu *et al* arXiv:2302.04505

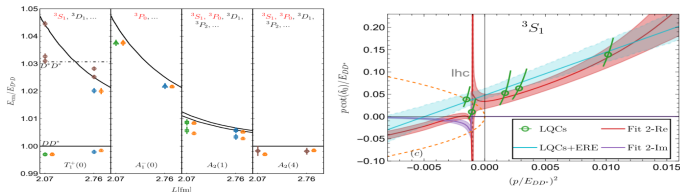
Long distance potential dominated by two pion exchange, not OPE.

Phase shifts extracted from long distance behaviour.

Shallow virtual bound state turning to a real bound state at physical m_π

Solutions: A plane-wave approach and modified LQC

- ✿ An effective field theory incorporating OPE with a plane wave basis expansion.



Lu Meng *et al* arXiv:2312.01930

Virtual bound states \Rightarrow Virtual resonances [$m_\pi \sim 280$ MeV]

- ✿ Modified 3-particle (Lüscher) Quantization Condition:

Hansen, Romero-Lopez, Sharpe, 2401.06609, Raposo, Hansen, 2311.18793

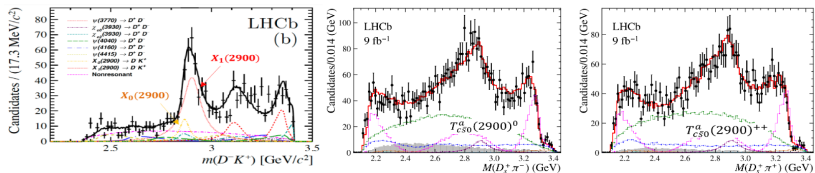
See a recent talk by Romero-Lopez [here](#)

A rigorous procedure, but demands multiple lattice inputs.

- $D\pi$ finite volume spectrum up to the $D\pi\pi$ threshold.
- Isovector DD finite volume spectrum up to the $DD\pi$ threshold.
- Isoscalar $DD\pi$ finite volume spectrum up to the $DD\pi\pi$ threshold.

Excited charmed-light and charmed-strange mesons

- Scalar D_0^* a broad feature in the $D\pi$ amplitudes, whereas a narrow D_{s0}^* below the DK threshold.
- Recent [LHCb] discoveries of T_{cs} [$X_1(2900)$, $X_0(2900)$], $T_{c\bar{s}0}(2900)^{0/++}$.



See talk by Liming Zhang

- A new framework of four quark systems with a charm quark and remaining light/strange quarks [$cs\bar{u}\bar{d}$, $cu\bar{s}\bar{d}$, $cd\bar{s}\bar{u}$].

LHCb discoveries

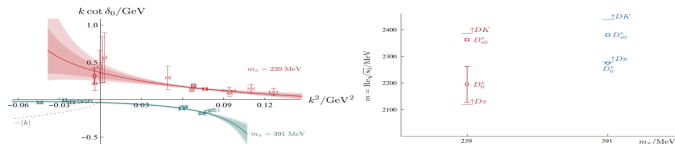
- A handful of lattice calculations (not explicitly exotic channels):

Mohler *et al* 1308.3175 (PRL), Lang *et al* 1403.8103, Bali *et al* 1706.01247, Gayer *et al* 2102.04973,

Mohler *et al* 1208.4059, Moir *et al* 1607.07093, Gregory *et al* 2106.15391, Yan *et al* 2312.01078

Recent lattice investigations

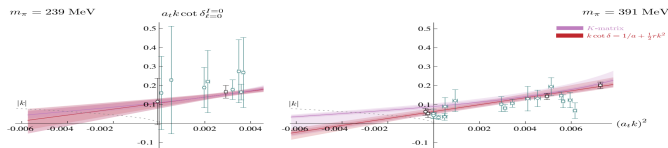
- Scalar charmed mesons and the $D\pi$ amplitudes,



Gayer *et al* 2102.04973

D_0^* pole real part consistently below that for D_{s0}^* for either m_π .

- Isoscalar $D\bar{K}$ scattering in s -wave (explicitly flavor exotic channel “ $cs\bar{q}_1\bar{q}_2$ ”):



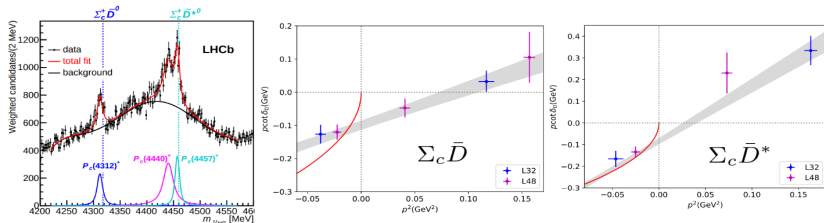
Cheung *et al* 2008.06432

Weak attraction indicating presence of a virtual state.

Pentaquarks, P_c in $J/\psi p$ final states

- Narrow pentaquark structures $P_c(4312)^+$, $P_c(4440)^+$, and $P_c(4457)^+$ in $J/\psi p$ final states. Features close below the $\Sigma_c \bar{D}$ and $\Sigma_c \bar{D}^*$

LHCb 1904.03947 (PRL)

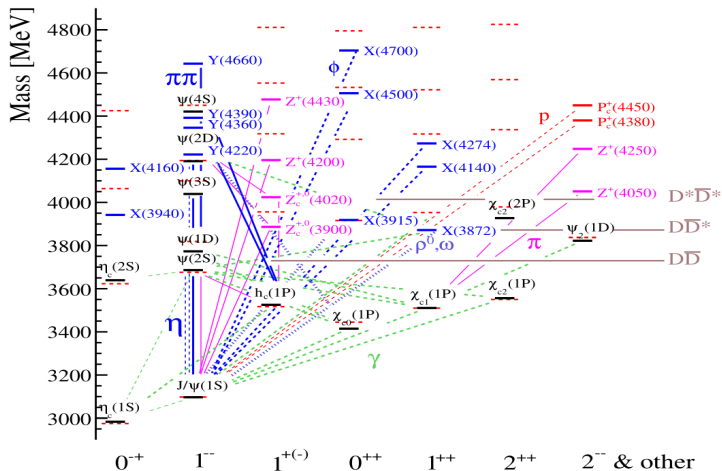


- Indications for shallow bound states in $\Sigma_c \bar{D}$ and $\Sigma_c \bar{D}^*$ from lattice. Coupling to $J/\psi p$ omitted in the analysis. $m_\pi \sim 294$ MeV.

Xing *et al* 2210.08555

- Evidence for $P_{cs}(4459)^0$ ($\bar{c}csud$) [LHCb]. No lattice investigation yet.

Charmonium



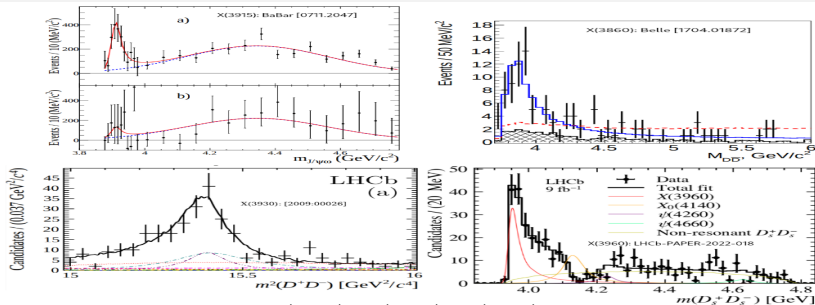
Rich energy spectrum. XYZ states.

$\bar{c}c$ picture works well for states below open charm threshold.

Olsen *et al* 1708.04012

No single description for states above the open charm threshold.

Focus: Scalar charmonium-like states



- Several likely related features, $X(3915)$, $X(3930)$, $X(3960)$.

Proximity to the $\bar{D}_s D_s$ threshold: Possible hidden strange content $[c\bar{s}c\bar{s}]$

\Rightarrow narrow width from $\bar{D}D$

- Several phenomenological studies supporting this:

Lebed Polosa 1602.08421, Chen *et al* 1706.09731, Bayar *et al* 2207.08490

- Another feature named as $X(3860)$ observed by Belle. No evidence from LHCb.

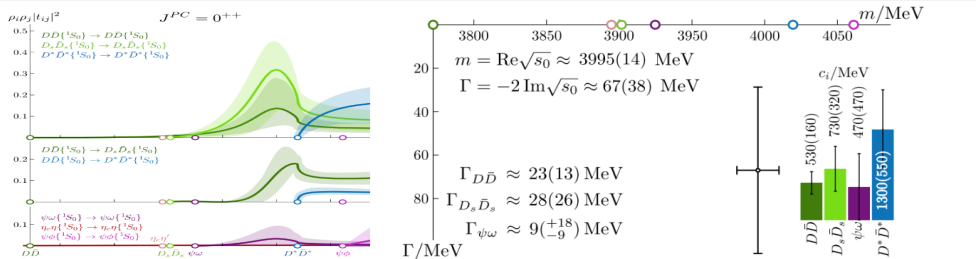
- Yet unknown $\bar{D}D$ bound state, predicted by models.

Gamermann *et al* 0612179, Hidalgo-Duque *et al* 1305.4487, Baru *et al* 1605.09649

- Such a $\bar{D}D$ bound state is supported by re-analysis of the exp. data.

Danilkin *et al* 2111.15033, Ji *et al* 2212.00631.

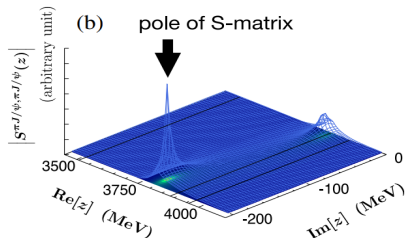
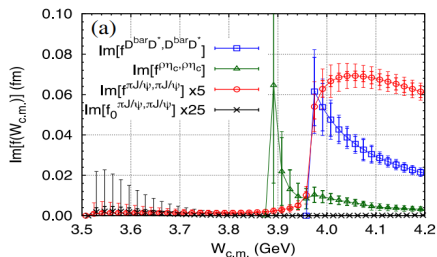
Recent lattice investigation by HSC



HSC 2309.14070, 2309.14071.

- Two-hadron channels considered: $\eta_c \eta$, $\eta_c \eta'$, $\bar{D}D$, $\bar{D}_s D_s$, $\psi\omega$, $\psi\phi$, $\bar{D}^* D^*$, $\chi_{c1} \eta$.
- Anisotropic lattice QCD ensembles : Hadron Spectrum Collaboration
 $m_\pi \sim 391 \text{ MeV}$, $m_K \sim 540 \text{ MeV}$, $m_D \sim 1852 \text{ MeV}$, $a_s \sim 0.12 \text{ fm}$
- In addition to conventional charmonium states, only a single scalar resonance below 4 GeV
 \Rightarrow with large coupling to all open charm channels.
 relation to X(3960) / X(3930) / X(3915) / $\chi_{c0}(3860)$ features ?
- Results in conflict with several other theoretical and experimental studies.
 Resolution: quark mass dependence ?

Charged charmonium-like states from lattice $[Z_c(3900)^+]$



HALQCD 1602.03465 (PRL).

- ❁ Lattice calculations from two different fronts:
Calculations based on Lüscher's formalism and using HALQCD approach

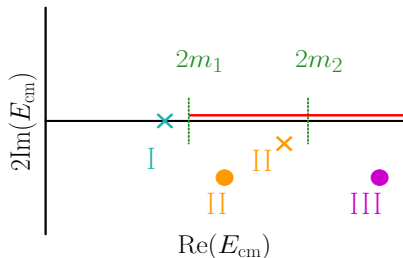
- ❁ HALQCD work: Coupled $J/\psi\pi\rho\eta_c\text{-}\bar{D}D^*$ scattering.
 $m_\pi \sim 400\text{-}700$ MeV, $a \sim 0.09$ fm
Strong coupling between $\bar{D}D^*$ and other two channels.
 $Z_c(3900)$ not a usual resonance, but a threshold cusp

- ❁ Lüscher's formalism: no robust supporting/excluding remarks for such a near threshold state.

Prelovsek *et al* 1405.7623, Chen *et al* 1403.1318, 1503.02371, CLQCD 1907.03371

Summary

- ✿ Compliments to the experimental efforts.
- ✿ Reported on lattice spectroscopic calculations involving charm quarks.
- ✿ Strong interaction stable hadrons: pretty well determined.
- ✿ Elastic resonances and near threshold states: Single channel
Several matured lattice determinations.
New challenges related left hand cuts.
- ✿ Inelastic resonances, exotic hadrons, etc.: Multiple channels.
Still a complex problem.
- ✿ Several prospective channels, FTFCF can contribute.



Thank you