

Lattice QCD investigation of mesons and tetraquark candidates

574. WE-Heraeus-Seminar: “Strong interactions in the LHC era”

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November 12, 2014



Goals, motivation (1)

- Compute the meson spectrum as fully as possible and study the structure of poorly understood candidates (scalar mesons, tetraquark candidates, ...) using lattice QCD:
 - *D* mesons (charm-light mesons, D , D^* , $D^{**} = \{D_0^*, D_1, D_2^*\}$, ...),
 - D_s mesons (charm-strange mesons, D_s , D_s^* , D_{s0}^* , D_{s1} , D_{s2}^* , ...),
 - charmonium (charm-charm mesons, η_c , J/ψ , ...),
 - “strangeonium” (strange-strange mesons, $a_0(980)$, $f_0(980)$, ...),
 - static-static-light-light systems (to improve the understanding of possibly existing tetraquarks).
 - Consider parity \pm , charge conjugation \pm , radial and orbital excitations.
- Lattice QCD \equiv from first principles (QCD), (ideally) all systematic errors quantified.

Goals, motivation (2)

- Why are such lattice investigations important?
 - **Some mesons are only poorly understood**
 - **lattice QCD is the perfect tool to clarify the situation:**
 - * Around 20 D , D_s and charmonium states labeled with “omitted from summary table”, i.e. vague experimental signals, experimental contradictions, states not well established, ...
 - * Example $X(3872)$ ($\bar{c}c$ state): mass not as expected from quark models; could be a D - D^* molecule, a bound diquark-antidiquark, ...
 - * Example $D_{s0}^*(2317)$, $D_{s1}(2460)$: masses significantly lower than expected from quark models, almost equal or even lower than the corresponding D mesons; could be tetraquarks, ...
 - Some mesons, e.g. D_s , η_c , J/ψ , have been measured experimentally with high precision and can also be computed on the lattice very accurately
 - ideal candidates to test QCD by means of lattice QCD.
 - Lattice QCD predictions could give valuable input for future experiments.



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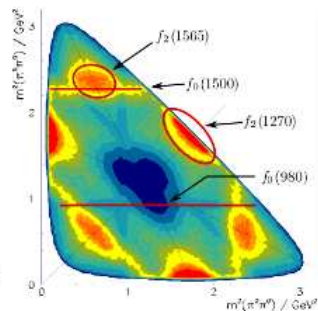
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Physics - Hadron Spectroscopy

Search for Gluonic Excitations

One of the main challenges of hadron physics is the search for gluonic excitations, i.e. hadrons in which the gluons can act as principal components. These gluonic hadrons fall into two main categories: glueballs, i.e. states where only gluons contribute to the overall quantum numbers, and hybrids, which consist of valence quarks and antiquarks as hadrons plus one or more excited gluons which contribute to the overall quantum numbers.

The additional degrees of freedom carried by gluons allow these hybrids and glueballs to have J^{PC} exotic quantum numbers. In this case mixing effects with nearby $q\bar{q}$ states are excluded and this makes their experimental identification easier. The properties of glueballs and hybrids are determined by the long-distance features of QCD and their study will yield fundamental insight into the structure of the QCD vacuum. Antiproton-proton annihilations provide a very favourable environment to search for gluonic hadrons.



Charmonium Spectroscopy

The charmonium spectrum can be calculated within the framework of non-relativistic potential models, EFT and LQCD. All 8 charmonium states below open charm threshold are known, but the measurements of their parameters and decays is far from complete (e.g. width and decay modes of h_c and $h_c(2S)$). Above threshold very little is known: on one hand the expected D- and F- wave states have not been identified (with the possible exception of the $\psi(3770)$, mostly $3D_1$), on the other hand the nature of the recently discovered X, Y, Z states is not known.

At full luminosity PANDA will collect several thousand $c\bar{c}$ states per day. By means of fine scans it will be possible to measure masses with an accuracy of the order of 100 keV and widths to 10% or better. PANDA will explore the entire energy region below and above the open charm threshold, to find the missing D- and F- wave states and unravel the nature of the newly discovered X, Y, Z states.

D Meson Spectroscopy

The recent discoveries of new open charm mesons at the BaBar, Belle and CLEO has attracted much interest both in the theoretical and experimental community, since the new states do not fit into the quark model predictions for heavy-light systems in contrast to the

Outline

- A brief introduction into lattice QCD hadron spectroscopy.
 - QCD (quantum chromodynamics).
 - Meson spectroscopy.
 - Lattice QCD.
- Some of our ongoing lattice projects:
 - (1) Spectrum of D , D_s , charmonium.
 - (2) Unstable mesons, tetraquarks, etc.
 - (3) Static-static-light-light tetraquarks.

QCD (quantum chromodynamics)

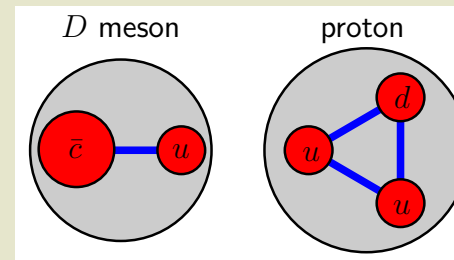
- Quantum field theory of **quarks** (six flavors u, d, s, c, t, b , which differ in **mass**) and **gluons**.
- Part of the standard model explaining the formation of hadrons (usually mesons = $q\bar{q}$ and baryons = $qqq/\bar{q}\bar{q}\bar{q}$) and their masses; essential for decays involving hadrons.
- Definition of QCD simple:

$$S = \int d^4x \left(\sum_{f \in \{u,d,s,c,t,b\}} \bar{\psi}^{(f)} \left(\gamma_\mu (\partial_\mu - iA_\mu) + m^{(f)} \right) \psi^{(f)} + \frac{1}{2g^2} \text{Tr} \left(F_{\mu\nu} F_{\mu\nu} \right) \right)$$

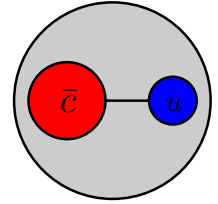
$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu - i[A_\mu, A_\nu].$$

- However, **no analytical solutions for low energy QCD observables, e.g. hadron masses, known**, because of the absence of any small parameter (i.e. perturbation theory not applicable).

→ **Solve QCD numerically by means of lattice QCD.**



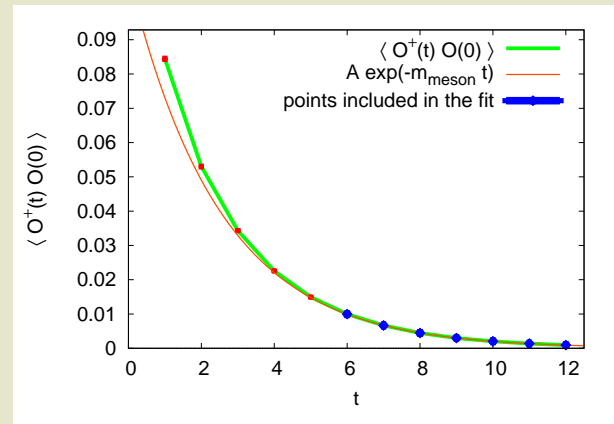
Meson spectroscopy



- Proceed as follows:
 - (1) Compute the temporal correlation function $C(t)$ of a mesonic $q\bar{q}$ operator O .
 - (2) Determine the meson mass of interest from the asymptotic exponential decay in time.
- Example: D meson mass m_D (valence quarks \bar{c} and u , $J^P = 0^-$),

$$O \equiv \int d^3r \bar{c}(\mathbf{r}) \gamma_5 u(\mathbf{r})$$

$$C(t) \equiv \langle \Omega | O^\dagger(t) O(0) | \Omega \rangle \stackrel{t \rightarrow \infty}{\propto} \exp(-m_D t).$$



Lattice QCD (1)

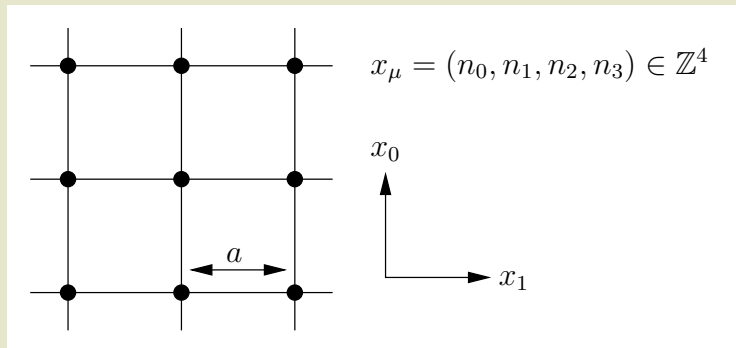
- To compute a temporal correlation function $C(t)$, use the path integral formulation of QCD,

$$\begin{aligned} C(t) &= \langle \Omega | O^\dagger(t) O(0) | \Omega \rangle = \\ &= \frac{1}{Z} \int \left(\prod_f D\psi^{(f)} D\bar{\psi}^{(f)} \right) DA_\mu O^\dagger(t) O(0) e^{-S[\psi^{(f)}, \bar{\psi}^{(f)}, A_\mu]}. \end{aligned}$$

- $|\Omega\rangle$: ground state/vacuum.
- $O^\dagger(t), O(0)$: functions of the quark and gluon fields (cf. previous slides).
- $\int (\prod_f D\psi^{(f)} D\bar{\psi}^{(f)}) DA_\mu$: integral over all possible quark and gluon field configurations $\psi^{(f)}(\mathbf{x}, t)$ and $A_\mu(\mathbf{x}, t)$.
- $e^{-S[\psi^{(f)}, \bar{\psi}^{(f)}, A_\mu]}$: weight factor containing the QCD action.

Lattice QCD (2)

- Numerical implementation of the path integral formalism in QCD:
 - Discretize spacetime with sufficiently small lattice spacing
 $a \approx 0.05 \text{ fm} \dots 0.10 \text{ fm}$
→ “continuum physics”.
 - “Make spacetime periodic” with sufficiently large extension
 $L \approx 2.0 \text{ fm} \dots 4.0 \text{ fm}$ (4-dimensional torus)
→ “no finite size effects”.



Lattice QCD (3)

- Numerical implementation of the path integral formalism in QCD:
 - After discretization the path integral becomes an ordinary multidimensional integral:

$$\int D\psi D\bar{\psi} DA \dots \rightarrow \prod_{x_\mu} \left(\int d\psi(x_\mu) d\bar{\psi}(x_\mu) dU(x_\mu) \right) \dots$$

- Typical present-day dimensionality of a discretized QCD path integral:
 - * x_μ : $32^4 \approx 10^6$ lattice sites.
 - * $\psi = \psi_A^{a,(f)}$: 24 quark degrees of freedom for every flavor ($\times 2$ particle/antiparticle, $\times 3$ color, $\times 4$ spin), 2 flavors.
 - * $U = U_\mu^{ab}$: 32 gluon degrees of freedom ($\times 8$ color, $\times 4$ spin).
 - * In total: $32^4 \times (2 \times 24 + 32) \approx \mathbf{83} \times \mathbf{10^6}$ dimensional integral.
- standard approaches for numerical integration not applicable
- sophisticated algorithms mandatory (stochastic integration techniques, so-called Monte-Carlo algorithms).

Spectrum of D , D_s , charmonium (1)

- In the following masses for D mesons, D_s mesons and charmonium states using quark-antiquark hadron creation operators, e.g. for D

$$\mathcal{O} \equiv \int d^3x \bar{c}(\mathbf{x}) \gamma_5 u(\mathbf{x}).$$

- **Accurate QCD results only for rather stable mesons, which are predominantly quark-antiquark states.**
- **Unstable mesons (e.g. D_0^* , $D_1(2430)$) or mesons, which might not predominantly be quark-antiquark states (e.g. the tetraquark candidates D_{s0}^* , D_{s1}), require more sophisticated techniques and computations:**
 - * **The correlation functions computed by means of lattice QCD provide the low-lying energy eigenvalues of the QCD Hamiltonian, which correspond to the masses of stable hadronic states (single or multi-particle).**
 - * **In lattice QCD the hadron creation operators may not be too different from the state, which is investigated.**

Spectrum of D , D_s , charmonium (2)

- First preliminary results of a large scale project.

[M. Kalinowski and M.W. [ETM Collaboration], PoS **Confinement10**, 303 (2012) [arXiv:1212.0403]]

[M. Kalinowski and M.W. [ETM Collaboration], Acta Phys. Polon. Supp. **6**, 991 (2013) [arXiv:1304.7974]]

[M. Kalinowski and M.W. [ETM Collaboration], PoS **LATTICE2013** [arXiv:1310.5513]]

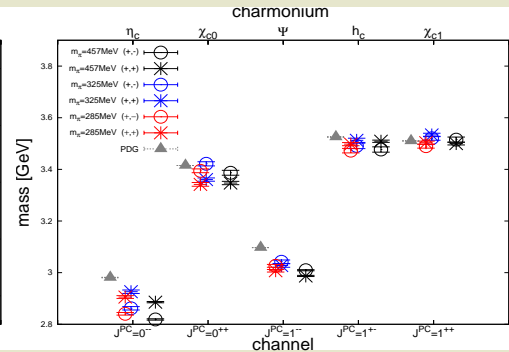
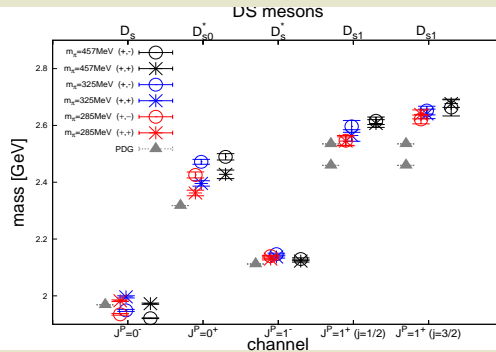
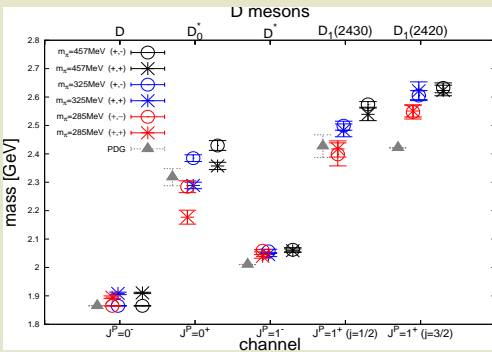
- D , D_s , charmonium states computed (in the plots from left to right):

– $J^P = 0^-$: D , D_s , η_c .

– $J^P = 0^+$: D_0^* , D_{s0}^* , χ_{c0} .

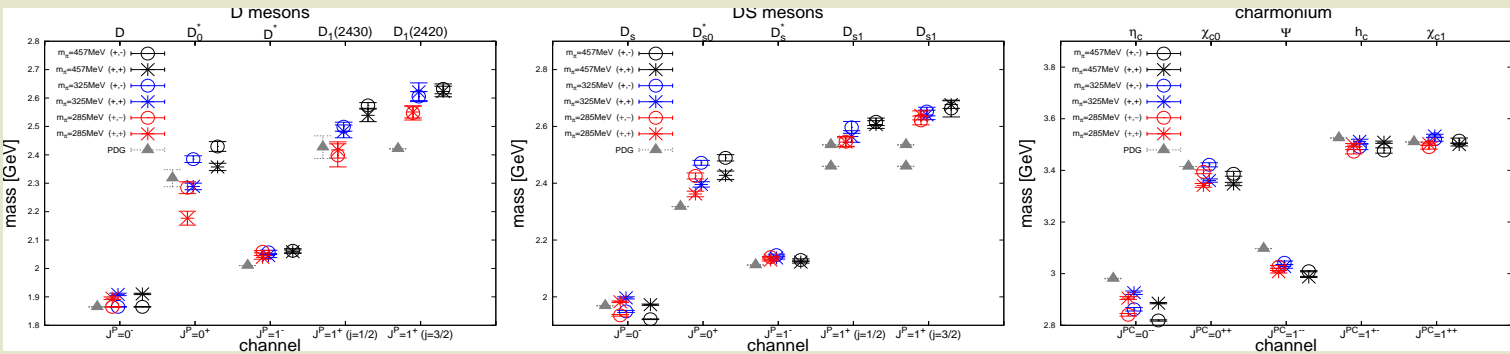
– $J^P = 1^-$: D^* , D_s^* , J/Ψ .

– $J^P = 1^+$: $D_1(2430)$, $D_1(2420)$, D_{s1} , D_{s1} , h_c , χ_{c1} .



Spectrum of D , D_S , charmonium (3)

- Experimental meson masses: gray points.
- Different lattice discretizations (circles and crosses) indicate that discretization errors are $\lesssim 2\%$ (will be removed in the near future).
- Different values of the light u/d quark mass (corresponding to $m_\pi = 285 \text{ MeV}$, 325 MeV , 457 MeV):
 - Some states are quite stable (**solid trustworthy results**), ...
 - ... others exhibit a clear dependence on the light quark mass (presumably unstable hadrons, mesonic molecules, tetraquarks containing light quarks; **further investigations necessary and ongoing**).



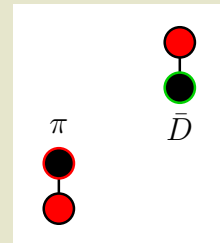
Unstable mesons, tetraquarks, etc. (1)

- Unstable mesons, e.g. $D_0^* \rightarrow D + \pi$, ...
For a proper treatment of such states, i.e. for a computation of their resonance mass and width using lattice QCD, one has to employ further hadron creation operators of two-meson structure.
- To study D_0^* ($J^P = 0^+$), in addition to a quark-antiquark operator

$$O_{D_0^*}^{q\bar{q}} = \int d^3x \bar{c}(\mathbf{x})u(\mathbf{x})$$

also a two-meson operator

$$O_{D_0^*}^{\text{two-meson}} = \underbrace{\left(\int d^3x \bar{c}(\mathbf{x})\gamma_5 l(\mathbf{x}) \right)}_{\equiv D} \underbrace{\left(\int d^3y \bar{l}(\mathbf{y})\gamma_5 l(\mathbf{y}) \right)}_{\equiv \pi}$$



($l = u, d$) is required (both generate the same quantum numbers $J^P = 0^+$, when applied to the vacuum).

Unstable mesons, tetraquarks, etc. (2)

- E.g. not clear, whether D_{s0}^* and D_{s1} are ordinary quark-antiquark states ... could be four quark states, for example mesonic molecules ($K-D$, ...), diquark-antidiquark states (tetraquarks), ...?

To investigate the structure of such mesons using lattice QCD one has to employ further hadron creation operators of mesonic molecule or of diquark-antidiquark structure.

Unstable mesons, tetraquarks, etc. (3)

- To study D_{s0}^* ($J^P = 0^+$), in addition to the quark-antiquark operator

$$O_{D_{s0}^*}^{q\bar{q}} = \int d^3x \bar{c}(\mathbf{x})s(\mathbf{x})$$

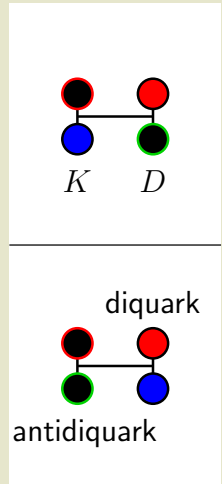
also four-quark operators

$$O_{D_0^*}^{\text{mesonic molecule}} = \int d^3x \underbrace{(\bar{c}(\mathbf{x})\gamma_5 l(\mathbf{x}))}_{\equiv D} \underbrace{(\bar{l}(\mathbf{x})\gamma_5 s(\mathbf{x}))}_{\equiv K}$$

$$O_{D_0^*}^{\text{diquark}} = \int d^3x \left(\epsilon^{abc} \bar{c}^b(\mathbf{x}) C \gamma_5 \bar{l}^{c,T}(\mathbf{x}) \right) \left(\epsilon^{ade} l^{d,T}(\mathbf{x}) C \gamma_5 s^e(\mathbf{x}) \right).$$

($l = u, d$) are required (both generate the same quantum numbers $J^P = 0^+$, when applied to the vacuum).

- Further examples of heavy mesons, which are tetraquark candidates: charmonium states $X(3872)$, $Z(4430)^\pm$, $Z(4050)^\pm$, $Z(4250)^\pm$, ...

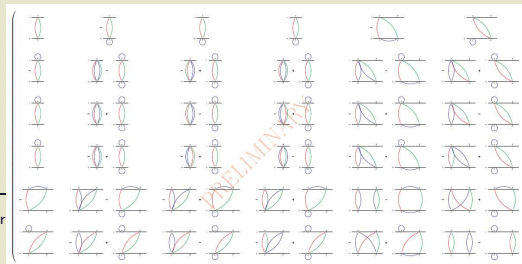


Unstable mesons, tetraquarks, etc. (4)

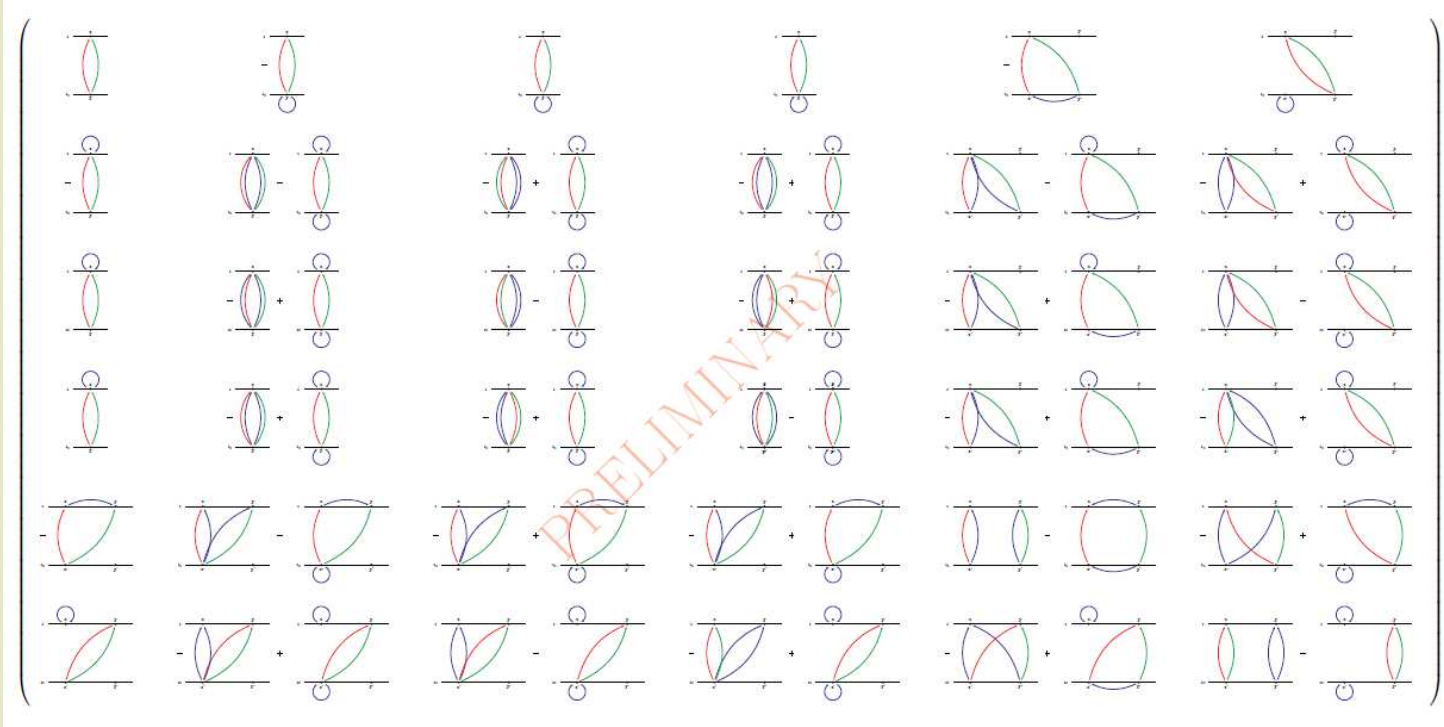
- When several operators are used one has to compute correlation matrices, not only a single correlation function.
- Many contributions (similar to Feynman diagrams, but with non-perturbative propagators), some of them very noisy, need to be computed rather precisely (different techniques required).
→ **Solid results require years of collaborative work.**
- Computations for several spatial volumes needed, to study resonance parameters.
- At the moment: preliminary results for $a_0(980)$ (" $a_0(980)$ is not a rather stable four-quark state. ").

[C. Alexandrou *et al.* [ETM Collaboration], JHEP **1304**, 137 (2013) [arXiv:1212.1418]]

[A. Abdel-Rehim *et al.*, arXiv:1410.8757]



Unstable mesons, tetraquarks, etc. (5)

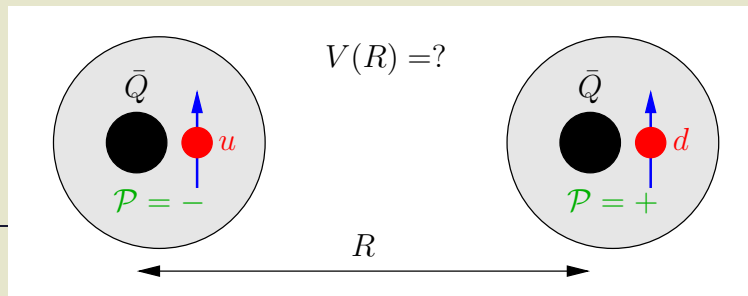


Heavy-heavy-light-light tetraquarks (1)

- Study possibly existing $\bar{Q}\bar{Q}qq$ and $\bar{Q}Q\bar{q}q$ tetraquark states ($q \in \{u, d, s, c\}$):
 - Use the static approximation for the heavy quarks $\bar{Q}\bar{Q}$ and $\bar{Q}Q$ (reduces the necessary computation time significantly).
 - Most appropriate for $\bar{Q}\bar{Q} \equiv \bar{b}\bar{b}$ and $\bar{Q}Q \equiv \bar{b}b$, e.g. $Z_b(10610)^+$ and $Z_b(10650)^+$.
 - Could also yield information about $\bar{Q}\bar{Q} \equiv \bar{c}\bar{c}$ and $\bar{Q}Q \equiv \bar{c}c$, e.g. $Z_c(3940)^\pm$ and $Z_c(4430)^\pm$.
- Proceed in two steps:
 - (1) Compute the potential of two heavy quarks $\bar{Q}\bar{Q}$ and $\bar{Q}Q$ in the background of two light quarks qq and $\bar{q}q$ by means of lattice QCD.
 - (2) Solve the non-relativistic Schrödinger equation for the relative coordinate of the heavy quarks $\bar{Q}\bar{Q}$ and $\bar{Q}Q$; a bound state would indicate a tetraquark state.

Heavy-heavy-light-light tetraquarks (2)

- Since heavy b quarks are treated in the static approximation, their spins are irrelevant (mesons are labeled by the spin of the light degrees of freedom j).
 - Consider only pseudoscalar/vector mesons ($j^P = (1/2)^-$, PDG: B, B^*) and scalar/pseudovector mesons ($j^P = (1/2)^+$, PDG: B_0^*, B_1^*), which are among the lightest static-light mesons.
 - Study the dependence of the mesonic potential $V(R)$ on
 - the “light” quark flavors u, d, s and/or c (isospin),
 - the “light” quark spin (the static quark spin is irrelevant),
 - the type of the meson S and/or P_- .
- Many different channels/quantum numbers ... attractive, repulsive ...

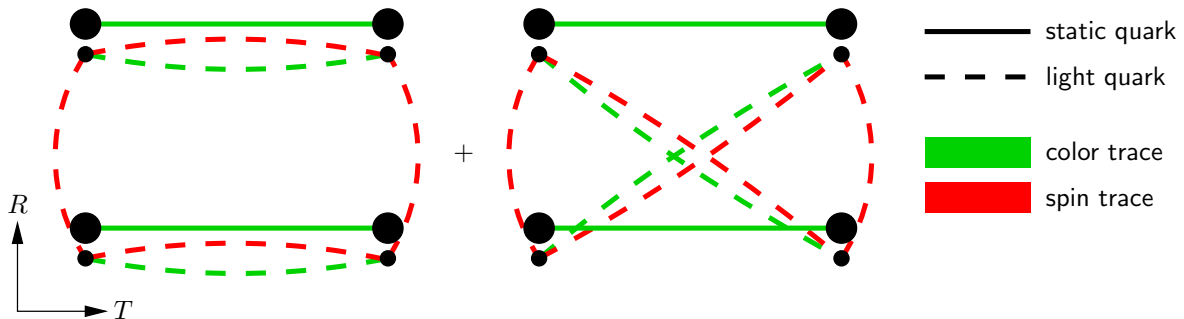


Heavy-heavy-light-light tetraquarks (3)

- In the following $\bar{Q}\bar{Q}qq$, i.e. “ BB ” (not $\bar{Q}\bar{Q}\bar{q}q$, i.e. “ $B\bar{B}$ ”).
- To extract the potential(s) of a given sector $(I, I_z, |j_z|, \mathcal{P}, \mathcal{P}_x)$, compute the temporal correlation function of the trial state

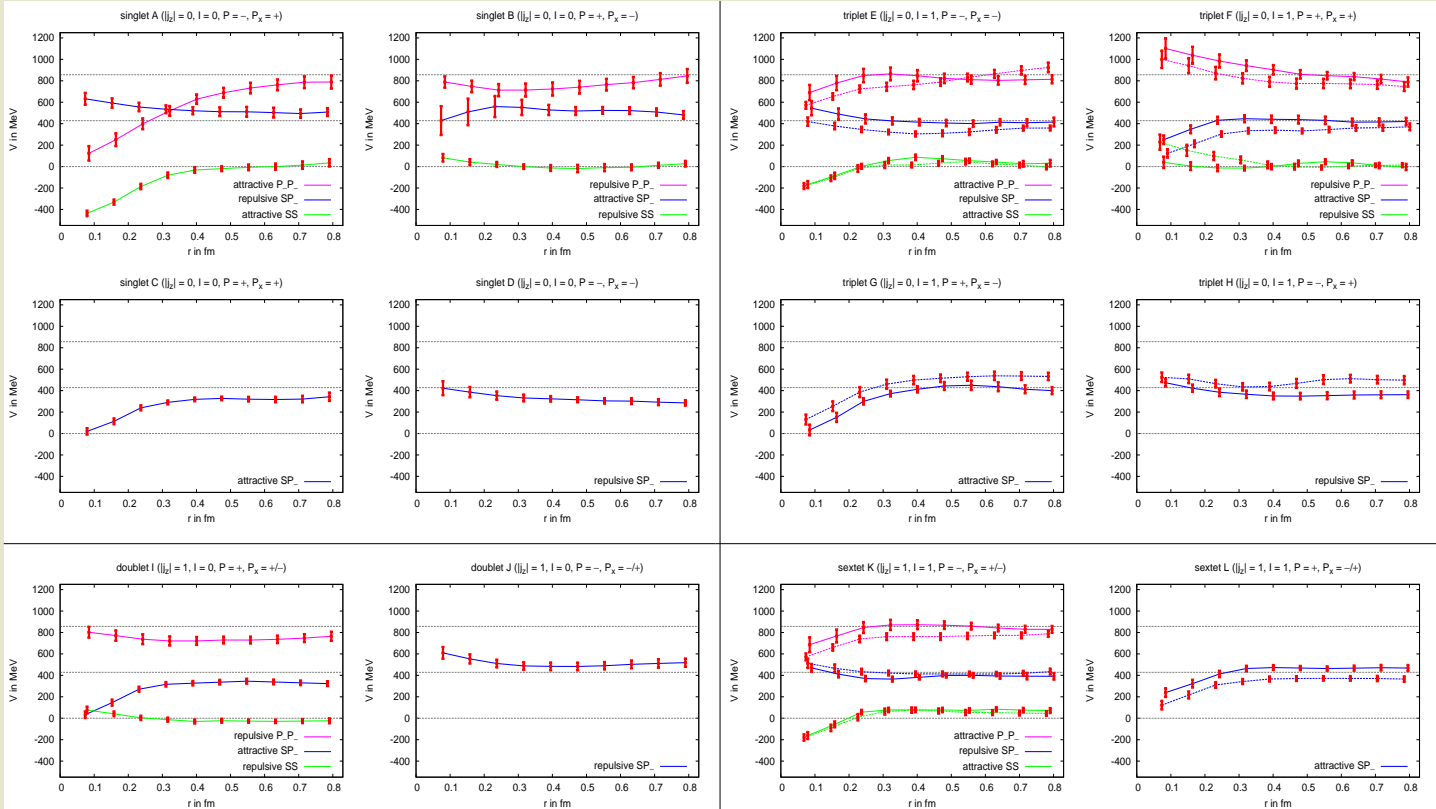
$$(\mathcal{C}\Gamma)_{AB} \left(\bar{Q}_C(-R/2) q_A^{(1)}(-R/2) \right) \left(\bar{Q}_C(+R/2) q_B^{(2)}(+R/2) \right) |\Omega\rangle.$$

- $\mathcal{C} = \gamma_0\gamma_2$ (charge conjugation matrix).
- $q^{(1)}q^{(2)} \in \{ud - du, uu, dd, ud + du, ss, cc\}$ (isospin I, I_z).
- Γ is an arbitrary combination of γ matrices (spin $|j_z|$, parity $\mathcal{P}, \mathcal{P}_x$).



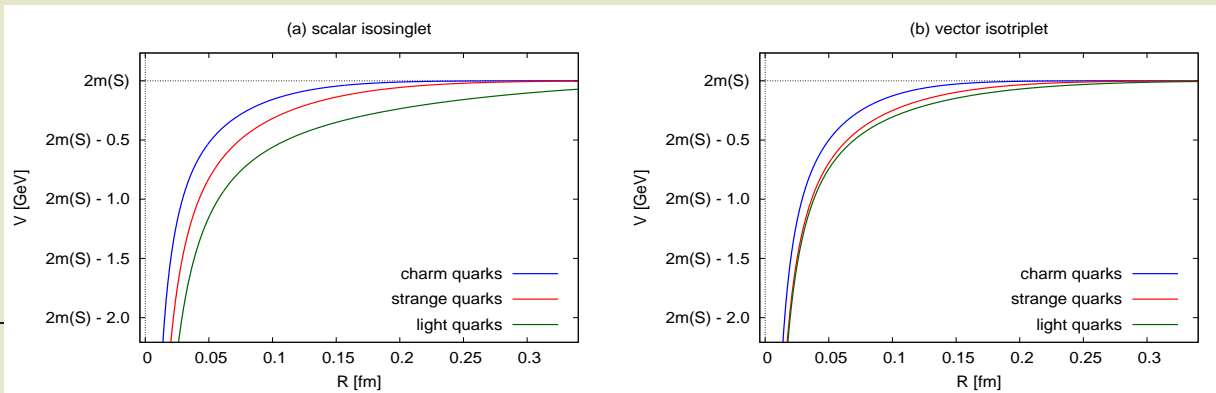
Heavy-heavy-light-light tetraquarks (4)

- $I = 0$ (left) and $I = 1$ (right); $|j_z| = 0$ (top) and $|j_z| = 1$ (bottom).



Heavy-heavy-light-light tetraquarks (5)

- Focus on the two attractive channels between ground state static-light mesons “ B and/or B^* ” (probably the best candidates to find a tetraquark):
 - Scalar isosinglet (more attractive):
 $qq = (ud - du)/\sqrt{2}$, $\Gamma = \gamma_5 + \gamma_0\gamma_5$,
 quantum numbers $(I, |j_z|, \mathcal{P}, \mathcal{P}_x) = (0, 0, -, +)$.
 - Vector isotriplet (less attractive):
 $qq \in \{uu, (ud + du)/\sqrt{2}, dd\}$, $\Gamma = \gamma_j + \gamma_0\gamma_j$,
 quantum numbers $(I, |j_z|, \mathcal{P}, \mathcal{P}_x) = (1, \{0, 1\}, -, \pm)$.
- Computations for $qq = ll, ss, cc$ ($l \in \{u, d\}$) to study the mass dependence.



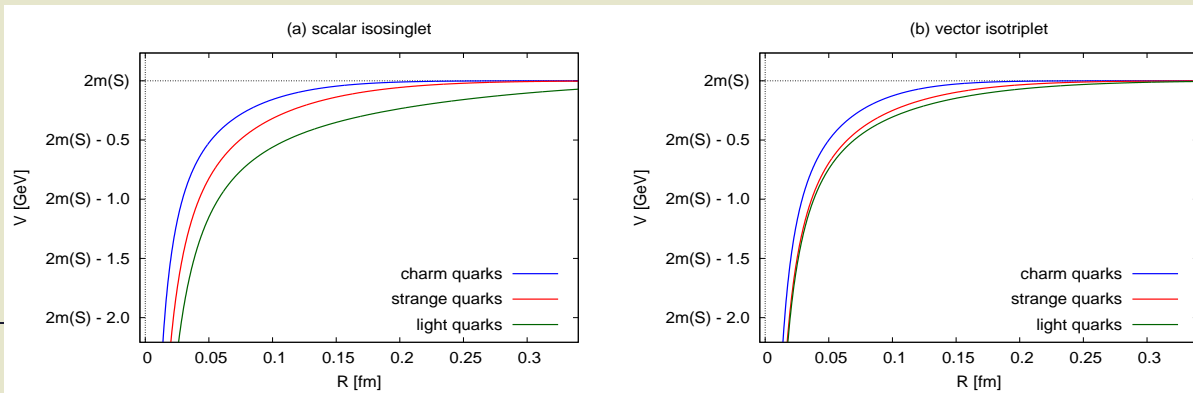
Heavy-heavy-light-light tetraquarks (6)

- Two competing effects:
 - The potential for light quarks is wider/deeper, i.e. favors the existence of a bound state (a tetraquark).
 - Heavier quarks correspond to heavier mesons ($m(B) < m(B_s) < m(B_c)$), which form more readily a bound state (a tetraquark), i.e. require a less wide/deep potential for a bound state.

[M.W., PoS LATTICE 2010, 162 (2010) [arXiv:1008.1538]]

[M.W., Acta Phys. Polon. Supp. 4, 747 (2011) [arXiv:1103.5147]]

[B. Wagenbach, P. Bicudo, M.W., arXiv:1411.2453]



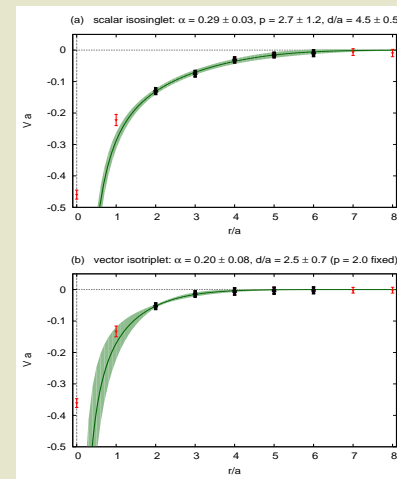
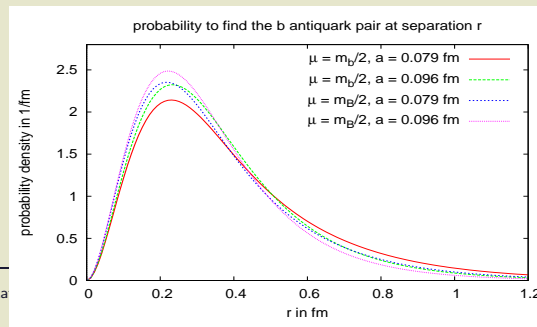
Static-static-light-light tetraquarks (7)

- Solve the non-relativistic Schrödinger equation for the relative coordinate of the heavy quarks $\bar{Q}\bar{Q}$,

$$\left(-\frac{1}{2\mu}\Delta + V(r) \right) \underbrace{\psi(\mathbf{r})}_{=R(r)/r} = E\psi(\mathbf{r}) \quad , \quad \mu = m(B_{(s,c)})/2;$$

a bound state, i.e. $E_0 < 0$, would be an indication for a tetraquark state.

- Clear indication for a bound state for the scalar isosinglet and $qq = ll$ (i.e. BB), binding energy $E \approx -50$ MeV, confidence level $\approx 2\sigma$.
- No binding for the vector isotriplet or for $qq = ss, cc$ (i.e. $B_s B_s, B_c B_c$).



Static-static-light-light tetraquarks (8)

- To quantify “no binding”, we list for each channel the factor, by which the effective mass μ in Schrödinger’s equation has to be multiplied, to obtain binding with confidence level 1σ and 2σ (the potential is not changed).

flavor	light		strange		charm	
	1σ	2σ	1σ	2σ	1σ	2σ
scalar isosinglet	0.8	1.0	1.9	2.2	3.1	3.2
vector isotriplet	1.9	2.1	2.5	2.7	3.4	3.5

- Factors ≤ 1.0 indicate binding.
- Light quarks (u/d) are unphysically heavy (correspond to $m_\pi \approx 340$ MeV); physically light u/d quarks are expected to yield stronger binding for the scalar isosinglet, might lead to binding also for the vector isotriplet (computations in progress).
- Mass splitting $m(B^*) - m(B) \approx 50$ MeV, neglected at the moment, is expected to weaken binding (coupled channel analysis in progress).

[P. Bicudo, M.W., Phys. Rev. D **87**, 114511 (2013) [arXiv:1209.6274]]

[B. Wagenbach, P. Bicudo, M.W., arXiv:1411.2453]

Static-static-light-light tetraquarks (9)

- At the moment only preliminary results for the experimentally more interesting case $\bar{Q}Q\bar{q}q$, i.e. “ $B\bar{B}$ ” (not $\bar{Q}\bar{Q}qq$, i.e. “ BB ”).
- $\bar{q}q = \bar{c}c$, “ $I = 1$ ”.
- Qualitative difference to $\bar{Q}\bar{Q}qq$: all channels are attractive (for $\bar{Q}\bar{Q}qq$ half of them are attractive, half of them are repulsive).
 - Can be understood by comparing the potential of $\bar{Q}Q$ and of $\bar{Q}\bar{Q}$ generated by one-gluon exchange.
 - For $\bar{Q}\bar{Q}$ the Pauli principle applied to qq implies either a symmetric (sextet) or an antisymmetric (triplet) color orientation of the static quarks corresponding to a repulsive or attractive interaction, respectively.
 - For $\bar{Q}Q$ no such restriction is present, i.e. all channels contain contributions of the attractive color singlet, which dominates the repulsive color octet.

Conclusions

- Rather stable mesons, which are predominantly quark-antiquark states (e.g. D , D_s):
 - Precise lattice QCD results are comparably simple to obtain.
- Instable mesons (resonances), tetraquark candidates (e.g. positive parity mesons $a_0(980)$, D_0^* , D_1 , D_{s0}^* , D_{s1}):
 - Rigorous lattice QCD results are extremely difficult to obtain.
 - **Lattice QCD computations with static quarks combined with model calculations could provide interesting qualitative and to some extent also quantitative insights.**

Spectrum of D , D_s , charmonium (A)

- In the following masses for D mesons, D_s mesons and charmonium states using quark-antiquark hadron creation operators.

Simulation setup

- Gauge link configurations generated with **2+1+1 dynamical quark flavors** by the European Twisted Mass Collaboration (ETMC).

ensemble	β	$(L/a)^3 \times T/a$	μ_l	μ_σ	μ_δ	a (fm)	m_π (MeV)	# of configurations
A30.32	1.90	$32^3 \times 64$	0.0030	0.150	0.190	0.086	284	1200
A40.32		$32^3 \times 64$	0.0040				324	800
A80.24		$24^3 \times 48$	0.0080				455	1700

- **Wilson twisted mass discretization** of quark fields:

(+) Automatic $\mathcal{O}(a)$ improvement of hadron masses.

(-) Parity and isospin are not anymore exact symmetries.

* u different from d , two possibilities for strange and charm quarks, s^+/s^- and c^+/c^- .

Spectrum of D , D_s , charmonium (B)

Meson creation operators (1)

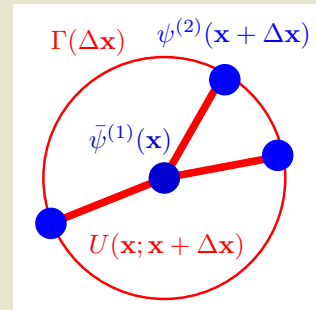
- Operators O , which generate the quantum numbers of a meson, when applied to the vacuum.
- Simple example (in a continuum notation): D meson, i.e. quantum numbers $J = 0$, $P = -$, $C = \pm 1$, $I = 1/2$, $\mathbf{p} = 0$,

$$O_{\gamma_5, \bar{c}u} \equiv \int d^3x \bar{c}(\mathbf{x}) \gamma_5 u(\mathbf{x}).$$

- General case: quantum numbers J , P , flavor, $\mathbf{p} = 0$,

$$O_{\Gamma, \bar{\psi}^{(1)}\psi^{(2)}} \equiv \int d^3x \bar{\psi}^{(1)}(\mathbf{x}) \int_{|\Delta\mathbf{x}|=R} d^3\Delta x U(\mathbf{x}; \mathbf{x} + \Delta\mathbf{x}) \Gamma(\Delta\mathbf{x}) \psi^{(2)}(\mathbf{x} + \Delta\mathbf{x}).$$

- $U(\mathbf{x}; \mathbf{x} + \Delta\mathbf{x})$ is a parallel transporter, $\Gamma(\Delta\mathbf{x})$ is a suitable linear combination of products of γ matrices and spherical harmonics.



Spectrum of D , D_S , charmonium (C)

Meson creation operators (2)

- General case: quantum numbers

J , P , flavor, $\mathbf{p} = 0$,

$$O_{\Gamma, \bar{\psi}^{(1)} \psi^{(2)}} \equiv \int d^3x \bar{\psi}^{(1)}(\mathbf{x}) \int_{|\Delta\mathbf{x}|=R} d^3\Delta x U(\mathbf{x}; \mathbf{x} + \Delta\mathbf{x}) \Gamma(\Delta\mathbf{x}) \psi^{(2)}(\mathbf{x} + \Delta\mathbf{x}).$$

	continuum			twisted mass lattice QCD			
	$\Gamma(\mathbf{n}), \text{pb}$	J	\mathcal{PC}	tb, (\pm, \mp)	tb, (\pm, \pm)	$O_h^S \times O_h^L \rightarrow O_h^J$	
1	γ_5	0	-+	pb	$i\gamma_5 \times$	$A_1 \otimes A_1$	A_1
2	$\gamma_0 \gamma_5$		-+	$i\gamma_5 \times$	pb		
3	$\mathbf{1}$		++	pb	$i\gamma_5 \times$		
4	γ_0		+-	$i\gamma_5 \times$	pb		
5	$\gamma_5 \gamma_1 \mathbf{n}_1$		--	$i\gamma_5 \times$	pb	$T_1 \otimes T_1$	
6	$\gamma_0 \gamma_5 \gamma_1 \mathbf{n}_1$		-+	pb	$i\gamma_5 \times$		
7	$\gamma_1 \mathbf{n}_1$		++	$i\gamma_5 \times$	pb		
8	$\gamma_0 \gamma_1 \mathbf{n}_1$		++	pb	$i\gamma_5 \times$		

Spectrum of D , D_s , charmonium (D)

Meson creation operators (3)

	continuum			twisted mass lattice QCD			
	$\Gamma(\mathbf{n}), \text{pb}$	J	\mathcal{PC}	tb, (\pm, \mp)	tb, (\pm, \pm)	$O_h^S \times O_h^L \rightarrow O_h^J$	
1	γ_1	1	--	$i\gamma_5 \times$	pb	$T_1 \otimes A_1$	T_1
2	$\gamma_0 \gamma_1$		--	pb	$i\gamma_5 \times$		
3	$\gamma_5 \gamma_1$		++	$i\gamma_5 \times$	pb		
4	$\gamma_0 \gamma_5 \gamma_1$		+-	pb	$i\gamma_5 \times$		
5	\mathbf{n}_1		--	pb	$i\gamma_5 \times$	$A_1 \otimes T_1$	
6	$\gamma_0 \mathbf{n}_1$		-+	$i\gamma_5 \times$	pb		
7	$\gamma_5 \mathbf{n}_1$		+-	pb	$i\gamma_5 \times$		
8	$\gamma_0 \gamma_5 \mathbf{n}_1$		+-	$i\gamma_5 \times$	pb		
9	$(\mathbf{n} \times \vec{\gamma})_1$		++	$i\gamma_5 \times$	pb	$T_1 \otimes T_1$	
10	$\gamma_0 (\mathbf{n} \times \vec{\gamma})_1$		++	pb	$i\gamma_5 \times$		
11	$\gamma_5 (\mathbf{n} \times \vec{\gamma})_1$		--	$i\gamma_5 \times$	pb		
12	$\gamma_0 \gamma_5 (\mathbf{n} \times \vec{\gamma})_1$		-+	pb	$i\gamma_5 \times$		
13	$\gamma_1 (2\mathbf{n}_1^2 - \mathbf{n}_2^2 - \mathbf{n}_3^2)$		--	$i\gamma_5 \times$	pb	$T_1 \otimes E$	
14	$\gamma_0 \gamma_1 (2\mathbf{n}_1^2 - \mathbf{n}_2^2 - \mathbf{n}_3^2)$		--	pb	$i\gamma_5 \times$		
15	$\gamma_5 \gamma_1 (2\mathbf{n}_1^2 - \mathbf{n}_2^2 - \mathbf{n}_3^2)$		++	$i\gamma_5 \times$	pb		
16	$\gamma_0 \gamma_5 \gamma_1 (2\mathbf{n}_1^2 - \mathbf{n}_2^2 - \mathbf{n}_3^2)$		+-	pb	$i\gamma_5 \times$		

Spectrum of D , D_S , charmonium (E)

Meson creation operators (4)

	continuum			twisted mass lattice QCD			
	$\Gamma(\mathbf{n}), \text{pb}$	J	\mathcal{PC}	tb, (\pm, \mp)	tb, (\pm, \pm)	$O_h^S \times O_h^L \rightarrow O_h^J$	
1	$\mathbf{n}_1^2 + \mathbf{n}_2^2 - 2\mathbf{n}_3^2$	2	++	pb	$i\gamma_5 \times$	$A_1 \otimes E$	E
2	$\gamma_0 \mathbf{n}_1^2 + \mathbf{n}_2^2 - 2\mathbf{n}_3^2$		-+	$i\gamma_5 \times$	pb		
3	$\gamma_5 \mathbf{n}_1^2 + \mathbf{n}_2^2 - 2\mathbf{n}_3^2$		-+	pb	$i\gamma_5 \times$		
4	$\gamma_0 \gamma_5 \mathbf{n}_1^2 + \mathbf{n}_2^2 - 2\mathbf{n}_3^2$		+−	$i\gamma_5 \times$	pb		
5	$(\gamma_1 \mathbf{n}_1 + \gamma_2 \mathbf{n}_2 - 2\gamma_3 \mathbf{n}_3)$		++	$i\gamma_5 \times$	pb	$T_1 \otimes T_1$	
6	$\gamma_0 (\gamma_1 \mathbf{n}_1 + \gamma_2 \mathbf{n}_2 - 2\gamma_3 \mathbf{n}_3)$		++	pb	$i\gamma_5 \times$		
7	$\gamma_5 (\gamma_1 \mathbf{n}_1 + \gamma_2 \mathbf{n}_2 - 2\gamma_3 \mathbf{n}_3)$		--	$i\gamma_5 \times$	pb		
8	$\gamma_0 \gamma_5 (\gamma_1 \mathbf{n}_1 + \gamma_2 \mathbf{n}_2 - 2\gamma_3 \mathbf{n}_3)$		-+	pb	$i\gamma_5 \times$		
1	$(\gamma_2 \mathbf{n}_1 + \gamma_1 \mathbf{n}_2)$	2	++	$i\gamma_5 \times$	pb	$T_1 \otimes T_1$	T_2
2	$\gamma_0 (\gamma_2 \mathbf{n}_1 + \gamma_1 \mathbf{n}_2)$		++	pb	$i\gamma_5 \times$		
3	$\gamma_5 (\gamma_2 \mathbf{n}_1 + \gamma_1 \mathbf{n}_2)$		--	$i\gamma_5 \times$	pb		
4	$\gamma_0 \gamma_5 (\gamma_2 \mathbf{n}_1 + \gamma_1 \mathbf{n}_2)$		-+	pb	$i\gamma_5 \times$		
5	$\gamma_1 (\mathbf{n}_2^2 - \mathbf{n}_3^2)$		--	$i\gamma_5 \times$	$i\gamma_5 \times$	$T_1 \otimes E$	
6	$\gamma_0 \gamma_1 (\mathbf{n}_2^2 - \mathbf{n}_3^2)$		--	pb	$i\gamma_5 \times$		
7	$\gamma_5 \gamma_1 (\mathbf{n}_2^2 - \mathbf{n}_3^2)$		++	$i\gamma_5 \times$	pb		
8	$\gamma_0 \gamma_5 \gamma_1 (\mathbf{n}_2^2 - \mathbf{n}_3^2)$		+−	pb	$i\gamma_5 \times$		

Spectrum of D , D_S , charmonium (F)

Meson creation operators (5)

- Computations are done with twisted basis quark fields. Such twisted basis operators are not able to generate defined parity and isospin. In particular $P = -$ and $P = +$ states mix. Their masses have to be determined from a single correlation matrix.
→ Technically difficult. Large statistical errors.
- Instead of local quark fields spatially extended quark fields (“smeared quark fields”) are used.
→ The overlap to the meson states of interest is then significantly larger, which drastically reduces statistical errors.
- Rotational symmetry is broken on a cubic lattice (replaced by symmetry under cubic rotations). Instead of an infinite number of irreducible angular momentum representations (labeled by $J = 0, 1, 2, 3, \dots$) there are only five different representations (A_1, T_1, E, T_2, A_2).
→ States with angular momentum $J \geq 4$ are extremely difficult to resolve.

Spectrum of D , D_s , charmonium (G)

Correlation matrices and extraction of meson masses (1)

- Lattice QCD computation of correlation matrices of meson creation operators

$$C_{\Gamma_j; \Gamma_k; \bar{\chi}^{(1)} \chi^{(2)}}(t) \equiv \langle \Omega | (S(O_{\Gamma_j, \bar{\chi}^{(1)} \chi^{(2)}}(t)))^\dagger S(O_{\Gamma_k, \bar{\chi}^{(1)} \chi^{(2)}}(0)) | \Omega \rangle$$

for each twisted mass sector characterized by

- flavor $\bar{\chi}^{(1)} \chi^{(2)}$,
- the cubic representation $O_h(J)$ (A_1 , T_1 , E , T_2),
- in case of charmonium also either \mathcal{C} or $\mathcal{C} \circ \mathcal{P}^{(\text{tm})}$.

→ Takes many months on modern HPC systems (LOEWE-CSC).

- For D and D_s mesons:
 - 8×8 correlation matrices for A_1 , E and T_2 , 16×16 for T_1 .
- For charmonium: similar, but more complicated due to \mathcal{C} or $\mathcal{C} \circ \mathcal{P}^{(\text{tm})}$.

Spectrum of D , D_s , charmonium (H)

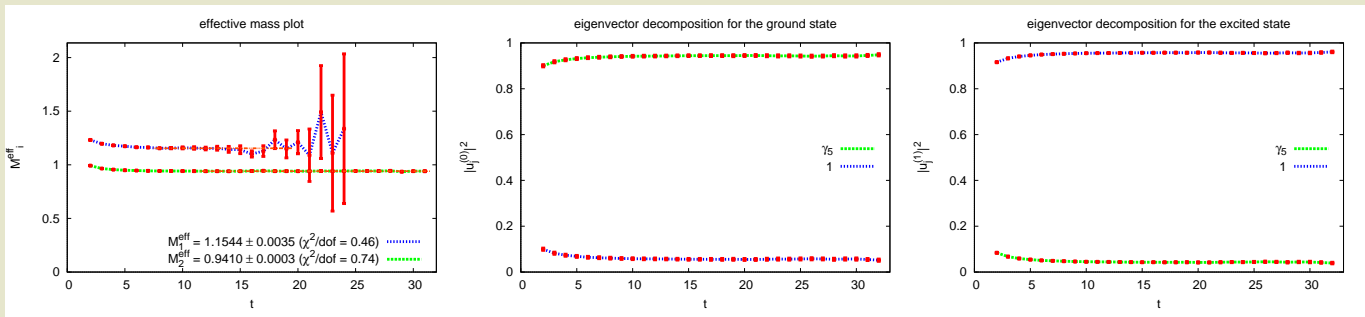
Correlation matrices and determination of meson masses (2)

- Example: mass of D_s ($J^P = 0^-$) and D_{s0}^* from a generalized eigenvalue problem and corresponding effective meson masses,

$$C(t)\vec{v}^{(n)}(t) = \lambda^{(n)}C(t_0)\vec{v}^{(n)}(t) \quad , \quad \vec{u}^{(n)}(t) = C(t_0)\vec{v}^{(n)}(t)$$

$$M_n^{\text{eff}}(t) \equiv \ln \left(\frac{\lambda^{(n)}(t)}{\lambda^{(n)}(t+1)} \right)$$

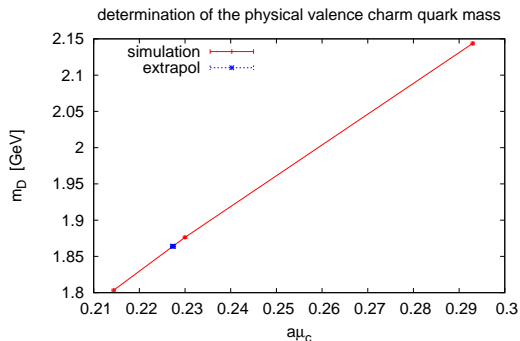
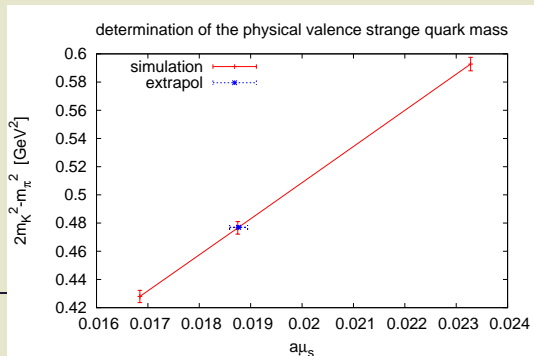
(C is a 2×2 correlation matrix containing the operators $\Gamma = \gamma_5$ and $\Gamma = 1$).



Spectrum of D , D_s , charmonium (I)

Determination of the physical strange and charm quark masses

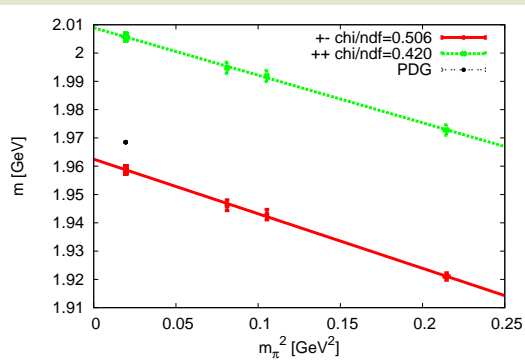
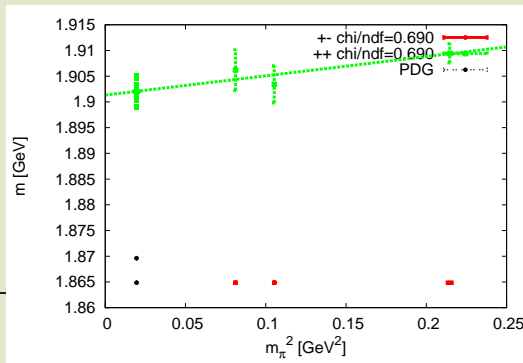
- Perform computations of meson masses at various strange and charm quark masses μ_s and μ_c (close to physical masses) and interpolate linearly.
- $\mu_s = \mu_s^{\text{physical}}$, where $2m_K^2 - m_\pi^2 = 2(m_K^{\text{physical}})^2 - (m_\pi^{\text{physical}})^2$.
 - The u/d quark mass is unphysically heavy due to technical reasons.
 - $m_K = m_K^{\text{physical}}$ would hence lead to an unphysically light s quark.
 - $2m_K^2 - m_\pi^2$ is independent of the u/d quark mass (in LO of χ PT).
- $\mu_c = \mu_c^{\text{physical}}$, where $m_D = m_D^{\text{physical}}$.



Spectrum of D , D_S , charmonium (J)

Extrapolation in the light u/d quark mass (1)

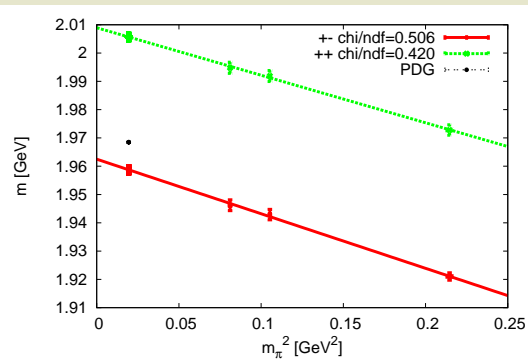
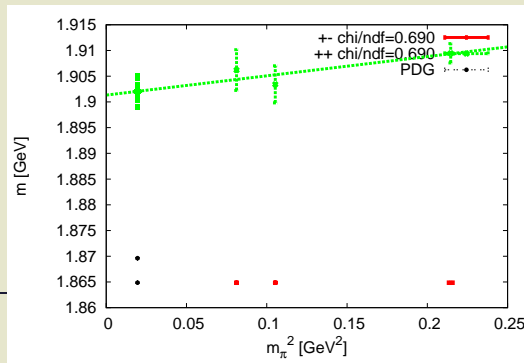
- Perform computations of meson masses at various unphysically heavy u/d quark masses ($m_\pi = 284$ MeV, 324 MeV, 455 MeV,) and interpolate linearly in m_π^2 ($m_\pi^2 \propto m_{u/d}$ in LO χ PT).



Spectrum of D , D_S , charmonium (K)

Extrapolation in the light u/d quark mass (2)

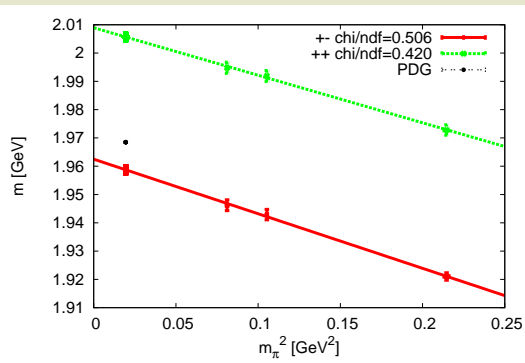
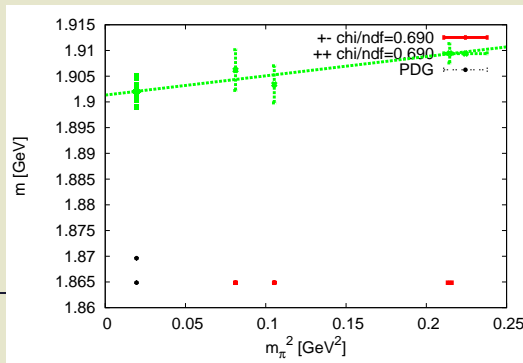
- Example: D meson (left plot), both $J^P = 0^-$.
 - Red dots: c^-u discretization, used to determine the c mass, i.e. no prediction, identical to m_{D^\pm} from PDG.
 - Green dots: c^-d discretization, difference to red dots ≈ 50 MeV due to twisted mass isospin breaking is an estimate of the lattice discretization errors at $a = 0.086$ fm (≈ 50 MeV amount to $\approx 2\%$ relative error).
 - Black dots: m_{D^\pm} and m_{D^0} from PDG, difference ≈ 5 MeV due to em and isospin effects (not considered in our QCD computations).



Spectrum of D , D_s , charmonium (L)

Extrapolation in the light u/d quark mass (3)

- Example: D_s meson (right plot), both $J^P = 0^-$.
 - Red dots: $c^- s^+$ discretization.
 - Green dots: $c^- s^-$ discretization.
 - Black dot: m_{D_s} from PDG, within the estimated lattice discretization errors of ≈ 50 MeV consistent with our prediction.
 - Negative slope in m_π , because of determination of μ_c^{physical} via $m_D = m_D^{\text{physical}}$ at unphysically heavy u/d quark mass (results in a lighter than physical μ_c for heavier than physical u/d quark mass).



Spectrum of D , D_s , charmonium (M)

- **Accurate QCD results only for rather stable mesons, which are predominantly quark-antiquark states** (e.g. the discussed D and D_s mesons).
- **Unstable mesons** (e.g. D_0^* , $D_1(2430)$) or **mesons, which might not predominantly be quark-antiquark states** (e.g. the tetraquark candidates D_{s0}^* , D_{s1}), require more sophisticated techniques and computations:
 - **The correlation functions computed by means of lattice QCD provide the low-lying energy eigenvalues of the QCD Hamiltonian, which correspond to the masses of stable hadronic states (single or multi-particle).**
 - **In lattice QCD the hadron creation operators may not be too different from the state, which is investigated.**

Spectrum of D , D_s , charmonium (N)

- First preliminary results of a large scale project.

[M. Kalinowski and M.W. [ETM Collaboration], PoS **Confinement10**, 303 (2012) [arXiv:1212.0403]]

[M. Kalinowski and M.W. [ETM Collaboration], Acta Phys. Polon. Supp. **6**, 991 (2013) [arXiv:1304.7974]]

[M. Kalinowski and M.W. [ETM Collaboration], PoS **LATTICE2013** [arXiv:1310.5513]]

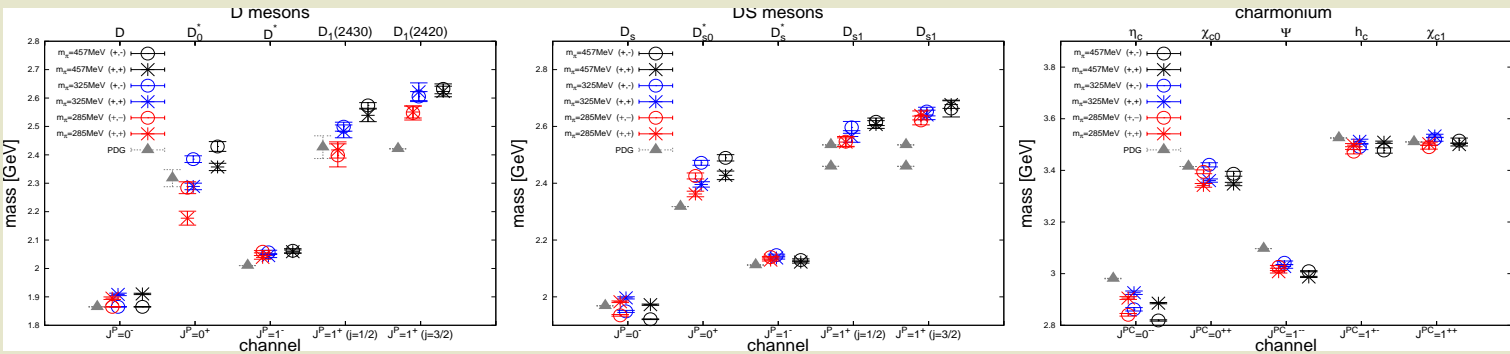
- D , D_s , charmonium states computed (in the plots from left to right):

– $J^P = 0^-$: D , D_s , η_c .

– $J^P = 0^+$: D_0^* , D_{s0}^* , χ_{c0} .

– $J^P = 1^-$: D^* , D_s^* , J/Ψ .

– $J^P = 1^+$: $D_1(2430)$, $D_1(2420)$, D_{s1} , D_{s1} , h_c , χ_{c1} .



Spectrum of D , D_s , charmonium (0)

- Experimental meson masses: gray points.
- Different lattice discretizations (circles and crosses) indicate that discretization errors are $\lesssim 2\%$ (will be removed in the near future).
- Different values of the light u/d quark mass (corresponding to $m_\pi = 284 \text{ MeV}$, 324 MeV , 455 MeV):
 - Some states are quite stable (**solid trustworthy results**), ...
 - ... others exhibit a clear dependence on the light quark mass (presumably unstable hadrons, mesonic molecules, tetraquarks containing light quarks; **further investigations necessary and ongoing**).

