Investigating heavy mesons and tetraquarks with lattice QCD

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• Compute the heavy meson spectrum as fully as possible and study the structure of poorly understood candidates using lattice QCD:
  – Heavy-light mesons and heavy-heavy mesons:
    * $D$ 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, $\eta_c, J/\psi$, ...),
  – Heavy-heavy tetraquark candidates:
    * 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, e.g. $D_s$, $\eta_c$, $J/\psi$, 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.
  - 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 $D_{s0}^*(2317)$, $D_{s1}(2460)$: masses significantly lower than expected from quark models, almost equal or even lower than the corresponding $D$ mesons; could be tetraquarks, ...
    - Lattice QCD could give valuable input for future experiments.
      * Prediction of a $bb\bar{u}\bar{d}$ tetraquark with $I(J^P) = 0(1^+)$. 

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 $J^P C$ exotic quantum numbers. In this case mixing effects with nearby $q ar{q}$ 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 $h_{c2}(2S)$). 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 communities, since the new states do not fit well into the quark model prediction for heavy-light systems, in contrast to the...
Outline

• A brief introduction to lattice QCD hadron spectroscopy.
  – QCD (quantum chromodynamics).
  – Meson spectroscopy.
  – Lattice QCD.

• Two of our lattice projects:
  (1) $D$ meson, $D_s$ meson and charmonium masses.
  (2) $\bar{b}bqq$ tetraquark candidates (ongoing).
Part 1: Introduction to lattice QCD
hadron spectroscopy
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:

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

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

- 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 $u$, $J^P = 0^-$),

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

$$C(t) \equiv \langle \Omega|O^\dagger(t)O(0)|\Omega\rangle \quad t \to \infty \quad \propto \exp \left( -m_D t \right).$$
Lattice QCD (1)

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

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

- $| \Omega \rangle$: ground state/vacuum.
- $O^\dagger(t), O(0)$: functions of the quark and gluon fields (cf. previous slides).
- $\int \left( \prod_f \mathcal{D} \psi^{(f)} \mathcal{D} \bar{\psi}^{(f)} \right) DA_\mu$: integral over all possible quark and gluon field configurations $\psi^{(f)}(x, t)$ and $A_\mu(x, t)$.
- $e^{-S[\psi^{(f)}, \bar{\psi}^{(f)}, A_\mu]}$: weight factor containing the QCD action.
• Numerical implementation of the path integral formalism in QCD:
  
  – Discretize spacetime with sufficiently small lattice spacing
    \[ a \approx 0.05 \text{ fm} \ldots 0.10 \text{ fm} \]
    \[ \rightarrow \text{“continuum physics”}. \]
  
  – “Make spacetime periodic” with sufficiently large extension
    \[ L \approx 2.0 \text{ fm} \ldots 4.0 \text{ fm (4-dimensional torus)} \]
    \[ \rightarrow \text{“no finite size effects”}. \]
Lattice QCD (3)

- Numerical implementation of the path integral formalism in QCD:
  - After discretization the path integral becomes an ordinary multidimensional integral:
    \[
    \int D\psi D\bar{\psi} DA \ldots \rightarrow \prod_{x_\mu} \left( \int d\psi(x_\mu) d\bar{\psi}(x_\mu) dU(x_\mu) \right) \ldots
    \]
  - Typical present-day dimensionality of a discretized QCD path integral:
    * \( x_\mu \): \( 32^4 \approx 10^6 \) 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: \( 32^4 \times (2 \times 24 + 32) \approx 83 \times 10^6 \) dimensional integral.
  \( \rightarrow \) standard approaches for numerical integration not applicable
  \( \rightarrow \) sophisticated algorithms mandatory (stochastic integration techniques, so-called Monte-Carlo algorithms).
Part 2: $D$ meson, $D_s$ meson and charmonium masses (quark-antiquark creation operators)

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

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

- **Accurate and solid 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.
$D, \ D_\text{s}, \text{ charmonium (2)}$

- Combined linear extrapolation in
  - the $u/d$ quark mass $m_{u,d} \propto m_{\pi}^2$ to $m_{\pi} = 135\ \text{MeV}$
    (horizontal axes in the plots)
  - in the squared lattice spacing $a^2$ to the continuum, i.e. $a = 0$
    (different curves/colors in the plots).

- Examples: $D_s$ meson (left plot), $\eta_c$ meson (right plot), both $J^P = 0^-$. 

- Different colors correspond to two different lattice discretizations and three different values of the lattice spacing.

- Perfect agreement between experimental results and the $u/d$ quark mass and continuum extrapolated lattice QCD results (combined statistical/systematic errors on the per mille level).
• Summary of lattice QCD results (blue and red boxes):

  - $D$ meson masses (left):
    $D, D^*_0, D^*, D_1(2430), D_1(2420), D^*_2$.

  - $D_s$ meson masses (center):
    $D_s, D_{s0}^*, D_s^*, D_{s1}(2460), D_{s1}(2536), D_{s2}^*$.

  - Charmonium masses (right):
    $\eta_c, \chi_{c0}, J/\Psi, \chi_{c1}, h_c, \chi_{c2}, \eta_{c2}, \Psi_2$.

(+) Computations with 2+1+1 dynamical quark flavors.
(+) Extrapolated to physically light $u/d$ quark masses.
(+) Extrapolated to the continuum.

(−) Only quark-antiquark creation operators, no four-quark operators at the moment.

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Comparison with existing experimental results (black boxes):

- Agreement for the majority of states.
- Tension/disagreement:
  * $D^*_s$, $D_{s1}(2460)$: tetraquark candidates
    ... might require four-quark creation operators.


* Radial excitations and higher orbital excitations (e.g. $\eta_c(2S)$, $J/\Psi(2S)$, $D^*_2$, $D_{s2}^*$)
  ... such excitations exhibit poor signals in lattice QCD, better statistics, i.e. longer computations required.
$D$, $D_s$, charmonium (5)

- Prediction of a couple of states, which have not yet been observed experimentally.
- Preparatory step for more advanced computations using also four-quark creation operators.
- Clear separation of the two $J^P = 1^+$ states
  
  $D_1(2430)$ (light spin $j \approx 1/2$)
  
  $D_1(2420)$ (light spin $j \approx 3/2$).


- Important to study semileptonic decays $B(\ast) \rightarrow D^{\ast\ast} + l + \nu$
  ($D^{\ast\ast}$: $J^P = 0^+, 1^+, 2^+$ $D$ mesons).

- Persistent conflict between experiment and theory ("1/2 versus 3/2 puzzle")
  ... experiment: decays to $j \approx 1/2$ more likely
  ... theory (QCD sum rules, quark models, lattice QCD): decays to $j \approx 3/2$ more likely
  ... both experiment and theory have problems (vague data, assumptions, etc.).

Part 3: $b\bar{b}qq$ tetraquark candidates
(creation operators with 2 static antiquarks and 2 quarks of finite mass)

\textbf{Basic idea}: Investigate the existence of heavy tetraquarks $\overline{b}bqq$ in two steps.

1. Compute potentials of two static antiquarks ($\overline{b}b$) in the presence of two lighter quarks ($qq \in \{ud, ss, cc\}$) using lattice QCD.

2. Check, whether these potentials are sufficiently attractive, to host a bound state by solving a corresponding Schrödinger equation. (\(\rightarrow\) This would indicate a stable $\overline{b}bqq$ tetraquark.)

\(\rightarrow\) \textbf{(1) + (2) \rightarrow Born-Oppenheimer approximation:}

- Proposed in 1927 for molecular and solid state calculations. 
- In our computations step (1) not quantum mechanics, but lattice QCD.
- Approximation valid, if \(m_q \ll m_b\) (most appropriate for \(qq = ud\)).
\( \bar{b}bqq \) tetraquarks (2)

**Born-Oppenheimer approximation, step (1)**

- Lattice QCD computation of \( \bar{b}b \) potentials \( V_{\bar{b}b}(r) \).

1. Use \( \bar{b}bqq \) creation operators

\[
O_{\bar{b}bqq} \equiv (C\Gamma)_{AB}(C\tilde{\Gamma})_{CD}\left(\bar{b}_C(-r/2)q_A^{(1)}(-r/2)\right)\left(\bar{b}_D(+r/2)q_B^{(2)}(+r/2)\right).
\]

* Different light quark flavors \( qq \in \{ud, ss, cc\} \).
* Different quark spin/parity.

→ Many different channels
  ... some attractive, some repulsive
  ... some correspond for large \( \bar{b}b \) separations to pairs of ground state mesons, some to excited mesons.

2. Compute temporal correlation functions.

3. Determine \( V_{\bar{b}b}(r) \) from the exponential decays of the correlation functions.

- $I = 0$ (left) and $I = 1$ (right); $|j_z| = 0$ (top) and $|j_z| = 1$ (bottom).
$\bar{b}\bar{b}qq$ tetraquarks (4)

- Two attractive channels corresponding to pairs of ground state mesons.

- Light quark mass dependence of these channels:
  wider and deeper for $qq = ud$ compared to $qq = ss$ compared to $qq = cc$.
**Born-Oppenheimer approximation, step (2)**

- Solve the Schrödinger equation for the relative coordinate $r$ of the two $\bar{b}$ quarks,
  
  \[
  \left( -\frac{1}{2\mu} \Delta + V_{\bar{b}\bar{b}}(r) \right) \psi(r) = E \psi(r), \quad \mu = \frac{m_b}{2};
  \]

  possibly existing bound states, i.e. $E < 0$, indicate $\bar{b}\bar{b}qq$ tetraquarks.

- A single bound state for one specific potential $V_{\bar{b}\bar{b}}(r)$ and light quarks $qq = ud$:
  
  - Binding energy $E = -93^{+47}_{-43}$ MeV, i.e. confidence level $\approx 2\sigma$.
  - Quantum numbers of the $\bar{b}bud$ tetraquark: $I(J^P) = 0(1^+)$.  

→ **Prediction of a tetraquarks.**

- No further bound states, in particular not for $qq = ss$ or $qq = cc$.

- **Experimental results for $\bar{b}\bar{b}qq$ would be very interesting ...**
Work in Progress:

- Including effects due to the $\bar{b}b$ spins (static quark spins are irrelevant).
  $\rightarrow$ Binding energy reduced, $\bar{b}bud$ tetraquark persists (preliminary).

- Investigation of the structure of the $\bar{b}bud$ tetraquark
  ... is it a mesonic molecule ... or a diquark-antidiquark pair?

- The experimentally simpler/theoretically harder case $\bar{b}b\bar{q}q$ (e.g. $Z_b(10610)^+, Z_b(10650)^+$).
  $\rightarrow$ First crude lattice results indicate the existence of an $I(J^P) = 1(1^+)$ $\bar{b}b\bar{d}u$ tetraquark, i.e. are consistent with the experimentally observed $Z_b^\pm$ states.