Computation of $B$ mesons and $b$ baryons with lattice QCD

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Outline

(1) Introduction to lattice computations, QCD and lattice QCD (≈ 15 minutes).

(2) Selected research results from the field of $B$ physics (≈ 25 minutes):
   - Masses of $B$ and $B_s$ mesons.
   - Masses of $b$ baryons.
   - Forces between $B$ mesons.
   - Semileptonic decays $B \rightarrow D^{**}$.

(3) Further research interests and planned research (≈ 5 minutes).
Part 1: Introduction to lattice computations, QCD and lattice QCD.
Lattice computations in QM (1)

- Introduce the basic principle of lattice computations via a simple example, the 1-dimensional harmonic oscillator in quantum mechanics.

- (Euclidean) action of the harmonic oscillator:

  \[ S[x] = \int dt \left( \frac{m}{2} \dot{x}(t)^2 + \frac{m\omega^2}{2} x(t)^2 \right). \]

- Goal: compute the average quadratic oscillation \( x^2 \) for the ground state \(|0\rangle\), i.e. \( \langle 0|x^2|0 \rangle \), by means of a lattice computation.

- Starting point: path integral formulation (equivalent to Schrödinger’s equation),

  \[ \langle 0|x^2|0 \rangle = \frac{1}{Z} \int Dx \ x^2 e^{-S[x]}, \quad Z = \int Dx \ e^{-S[x]}. \]

  - \( \int Dx \): integral over all possible paths \( x(t) \), i.e. an integral over a function space (= “integral over infinitely many variables”).

  - \( e^{-S[x]} \): weight factor containing the action of the harmonic oscillator.
Lattice computations in QM (2)

• Starting point: path integral formulation (equivalent to Schrödinger’s equation),
\[
\langle 0 | x^2 | 0 \rangle = \frac{1}{Z} \int Dx \; x^2 e^{-S[x]}, \quad Z = \int Dx \; e^{-S[x]}.
\]

• Discretize and compactify time:
\[t \in \mathbb{R} \rightarrow t_j = j \times \Delta t, \quad j = 0, 1, \ldots, N - 1\]
\[\rightarrow \text{path integral reduced to an ordinary multi-dimensional integral, i.e.}\]
\[
\int Dx \; e^{-S[x]} \rightarrow \int \left( \prod_{j=0}^{N-1} dx(t_j) \right) e^{-S[x(t_0), \ldots, x(t_{N-1})]}.
\]

• Solve this multi-dimensional by means of a (high performance) computer.
“Standard model of particle physics”

- Four fundamental forces, which correspond to gauge bosons.
- Matter: six types of quarks and six types of leptons.
- QCD (quantum chromodynamics): quarks and gluons and their interactions.
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 (mesons = \(q\bar{q}\), baryons = \(qqq/\bar{q}\bar{q}\bar{q}\)) and their masses; essential for decays involving hadrons.

- Definition of QCD by means of an action 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).

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Lattice QCD (1)

- Goal: compute QCD observables, e.g. hadron masses, from first principles with controllable systematic error.

- Use the path integral formulation of QCD,

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

- \( \langle \ldots \rangle \): ground state/vacuum expectation value.

- \( \mathcal{O}(\psi(f), \bar{\psi}(f), A_\mu) \): function of the quark and gluon fields, which can be related to an observable, e.g. a specific meson/baryon mass.

- \( \int (\prod_f D\psi(f) \, D\bar{\psi}(f)) DA_\mu \): integral over all possible quark and gluon field configurations \( \psi(f)(x, t) \) and \( A_\mu(x, t) \).

- \( e^{-S[x]} \): weight factor containing the QCD action.

Note that this path integral is analogous to the quantum mechanical example,

\[
\langle 0 | x^2 | 0 \rangle = \frac{1}{Z} \int Dx \, x^2 e^{-S[x]}. 
\]
Lattice QCD (2)

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

\[ x_\mu = (n_0, n_1, n_2, n_3) \in \mathbb{Z}^4 \]
Lattice QCD (3)

- Numerical implementation of the path ...
  - Quark fields:
    * Action (in the continuum):
      \[ S_{E,\text{quarks}} = \int d^4x \sum_f \bar{\psi}^{(f)}(x) \left( \gamma_\mu \left( \partial_\mu - iA_\mu \right) + m_f \right) \psi^{(f)}(x). \]
    * “Direct discretization” of the quark fields \( \psi^{(f)} \), i.e. quark fields are defined on the lattice sites.
    * Conceptually more difficult, high performance computer systems needed:
      - Fermion doubling (cf. my previous presentation).
      - Chiral symmetry explicitly broken.
      - Simulations at physically realistic values of the \( u \) and \( d \) quark masses extremely computer time consuming.
      - Discretization errors proportional to the lattice spacing \( a \), i.e. rather large discretization errors.
Lattice QCD (4)

- 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.
    * \( U = U^{ab}_\mu \): 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.

→ standard approaches for numerical integration not applicable
→ sophisticated algorithms mandatory (stochastic integration techniques, so-called Monte-Carlo algorithms).
Twisted mass lattice QCD, ETMC

- Discretizing the QCD action is not unique.
- **Twisted mass lattice QCD** is a specific lattice discretization of QCD:
  - Advantages of twisted mass lattice QCD:
    (+) Automatic $\mathcal{O}(a)$ improvement of physical observables
    $\rightarrow$ lattice discretization errors due to fermions (quarks) do not appear linearly in the small lattice spacing $a$, only quadratically.
    (+) Compared to certain other lattice discretizations rather cheap
    $\rightarrow$ large lattice extensions and small lattice spacings feasible.
- The **European Twisted Mass Collaboration** (ETMC), a collaboration of more than twenty European universities and research institutes, of which I am a member, successfully uses this this discretization for already a couple of years to perform large scale computations of QCD with 2 quark flavors; recently we have started a similar major project to simulate 2+1+1 quark flavors.

Marc Wagner, “Computation of $B$ mesons and $b$ baryons with lattice QCD”, January 20, 2011
Part 2: Selected research results from the field of $B$ physics.
**B physics, B mesons, b baryons (1)**

- **B physics**, typical questions: properties of **B** mesons and **b** baryons, e.g. masses, investigations of their decays; ...
  - **B mesons**: bound quark antiquark pairs, where one of the quarks is a heavy “bottom” or **b** quark, the other is a light **u**, **d** or **s** quark.
  - **b baryons**: bound systems of three quarks/antiquarks, where one of the quarks is a heavy **b** quark, the remaining two are light **u**, **d** or **s** quarks.

<table>
<thead>
<tr>
<th>quark</th>
<th>mass in MeV/c²</th>
<th>electrical charge</th>
</tr>
</thead>
<tbody>
<tr>
<td>up down</td>
<td>1.5...3.3</td>
<td>+2/3e</td>
</tr>
<tr>
<td></td>
<td>3.5...6</td>
<td>−1/3e</td>
</tr>
<tr>
<td>strange</td>
<td>104^{+26}_{−34}</td>
<td>−1/3e</td>
</tr>
<tr>
<td>charm</td>
<td>1270^{+70}_{−11}</td>
<td>+2/3e</td>
</tr>
<tr>
<td>bottom</td>
<td>4200^{+170}_{−70}</td>
<td>−1/3e</td>
</tr>
<tr>
<td>top</td>
<td>170900 ± 1800</td>
<td>+2/3e</td>
</tr>
</tbody>
</table>

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$B$ physics, $B$ mesons, $b$ baryons (2)

- Discovery of the $b$ quark 1977.
- Present-day experiments:
  - BaBar experiment, SLAC (USA).
  - Belle experiment, KEK (Japan).
  - LHCb experiment, CERN (Switzerland).
  - ...

\[ B\text{ meson: } B^+ \quad b\text{ baryon: } \Lambda_b^0 \]
Masses of $B$ and $B_s$ mesons (1)

- $B/B_s$ meson:
  - Bound quark antiquark pair (a heavy $b$ quark and a light $u$, $d/s$ quark).
  - “Hydrogen atom of QCD”: a light particle ($u$, $d$, or $s$) “orbits” a heavy particle ($\bar{b}$).
  - States are characterized by:
    * Total angular momentum/spin of the light degrees of freedom $j$ (light quarks and gluons); we perform computations in the limit $m_B \to \infty$ (static limit), which amounts to neglecting hyperfine splitting; hyperfine splitting is “reincluded” at the end.
    * Parity $\mathcal{P}$.
    * Radial quantum number; in the following, however, mostly ground states in the corresponding $j^\mathcal{P}$ sectors.

Consequently, states are labeled by $j^\mathcal{P}$.
Masses of $B$ and $B_S$ mesons (2)

- Compute static-light meson masses ($B/B_S$ mesons with $m_b \to \infty$) for different light $u/d$ quark masses and different lattice spacings:
  - Different $u/d$ quark masses to extrapolate to the physical $u/d$ quark mass (due to technical reasons $m_\pi^{(\text{lattice})} \gtrsim 300$ MeV, $m_\pi^{\text{physical}} \approx 135$ MeV).
  - Different lattice spacings to extrapolate to the continuum.
  - Horizontal axis: pion mass $(m_\pi^{(\text{lattice})})^2$.
  - Vertical axis: $M(j^P) - m_B$ mass difference between radially and orbitally excited $B$ mesons ($B_0^*, B_1^*, B_1, B_2^*$, ...) and the ground state $B$ meson ($B^+/B^0/B^* \equiv j^P = (1/2)^{-}$) ... analogous for $B_S$ mesons.
Masses of $B$ and $B_{s}$ mesons (3)

- Summary of the computed static-light meson spectrum:

<table>
<thead>
<tr>
<th>$j^P$</th>
<th>alternative notation</th>
<th>$B$ mesons ($\bar{b}u$ or $\bar{b}d$): $M($meson$) - M(B)$ in MeV</th>
<th>$B_{s}$ mesons ($\bar{b}s$): $M($meson$) - M(B_{s})$ in MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1/2)^+$</td>
<td>$P_-$</td>
<td>406(19)</td>
<td>413(12)</td>
</tr>
<tr>
<td>$(3/2)^+$</td>
<td>$P_+</td>
<td>516(18)</td>
<td>504(12)</td>
</tr>
<tr>
<td>$(3/2)^-$, $(5/2)^-$</td>
<td>$D_{\pm}$</td>
<td>870(27)</td>
<td>770(26)</td>
</tr>
<tr>
<td>$(5/2)^-$</td>
<td>$D_+</td>
<td>930(28)</td>
<td>960(24)</td>
</tr>
<tr>
<td>$(5/2)^+$, $(7/2)^+$</td>
<td>$F_{\pm}$</td>
<td>1196(30)</td>
<td>1179(37)</td>
</tr>
<tr>
<td>$(1/2)^-$</td>
<td>$S^*$</td>
<td>755(16)</td>
<td>751(26)</td>
</tr>
</tbody>
</table>

- Motivation/achievements:
  - Continuum limit (among the first).
  - Dependence on the light $u/d$ sea quark mass (for the first time).
  - Valuable input for model builders (e.g. no reversal of $M(P_-)$ and $M(P_+)$, ...).
Masses of $B$ and $B_s$ mesons (4)

- Comparison to experimental results:
  - Extrapolation to the physical (finite) $b$ quark mass $m_B \approx 4200$ MeV by means of rather precise experimental results for $c$ quarks, i.e. $D$ mesons (amounts to “reincluding” hyperfine splitting):

<table>
<thead>
<tr>
<th>name</th>
<th>lattice</th>
<th>experiment</th>
<th>name</th>
<th>lattice</th>
<th>experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B_0^*$</td>
<td>443(21)</td>
<td></td>
<td>$B_{s0}^*$</td>
<td>391(8)</td>
<td></td>
</tr>
<tr>
<td>$B_1^*$</td>
<td>460(22)</td>
<td></td>
<td>$B_{s1}^*$</td>
<td>440(8)</td>
<td></td>
</tr>
<tr>
<td>$B_1$</td>
<td>530(12)</td>
<td>444(2)</td>
<td>$B_{s1}$</td>
<td>526(8)</td>
<td>463(1)</td>
</tr>
<tr>
<td>$B_2^*$</td>
<td>543(12)</td>
<td>464(5)</td>
<td>$B_{s2}^*$</td>
<td>539(8)</td>
<td>473(1)</td>
</tr>
<tr>
<td>$B_J^*$</td>
<td>418(8)</td>
<td></td>
<td>$B_{sJ}^*$</td>
<td></td>
<td>487(15)</td>
</tr>
</tbody>
</table>

- Difference between lattice and experimental results: scale setting problem?

[K. Jansen, C. Michael, A. Shindler and M.W. [ETM Collaboration], JHEP 0812, 058 (2008)]
[C. Michael, A. Shindler and M.W. [ETM Collaboration], JHEP 1008, 009 (2010)]
Masses of $b$ baryons (1)

- $b$ baryon: bound system of three quarks/antiquarks (a heavy $b$ quark and two light $u$, $d$ or $s$ quarks).
- Computation of masses similar to that of $B$ and $B_s$ mesons.
- Summary of the computed static-light baryon spectrum:

<table>
<thead>
<tr>
<th>$j^P$</th>
<th>$I$</th>
<th>$S$</th>
<th>name</th>
<th>$m(\text{baryon}) - m(B)$ in MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>0$^+$</td>
<td>0</td>
<td>0</td>
<td>$\Lambda^0_b$</td>
<td>434(46)</td>
</tr>
<tr>
<td>1$^+$</td>
<td>1</td>
<td>0</td>
<td>$\Sigma_b/\Sigma_b^*$</td>
<td>671(46)/632(39)</td>
</tr>
<tr>
<td>0$^-$</td>
<td>0</td>
<td>0</td>
<td>$-$</td>
<td>1389(113)</td>
</tr>
<tr>
<td>1$^-$</td>
<td>1</td>
<td>0</td>
<td>$-$</td>
<td>1008(92)/1014(79)</td>
</tr>
<tr>
<td>0$^+$</td>
<td>1/2</td>
<td>-1</td>
<td>$\Xi_b^-$</td>
<td>630(41)/677(36)</td>
</tr>
<tr>
<td>1$^+$</td>
<td>1/2</td>
<td>-1</td>
<td>$-$</td>
<td>789(45)/798(49)</td>
</tr>
<tr>
<td>0$^-$</td>
<td>1/2</td>
<td>-1</td>
<td>$-$</td>
<td>1200(90)/1262(77)</td>
</tr>
<tr>
<td>1$^-$</td>
<td>1/2</td>
<td>-1</td>
<td>$-$</td>
<td>1233(58)/1285(69)</td>
</tr>
<tr>
<td>1$^+$</td>
<td>0</td>
<td>-2</td>
<td>$\Omega_b^-$</td>
<td>903(42)</td>
</tr>
<tr>
<td>1$^-$</td>
<td>0</td>
<td>-2</td>
<td>$-$</td>
<td>1315(79)</td>
</tr>
</tbody>
</table>
Masses of \( b \) baryons (2)

- Comparison to experimental results:
  - Extrapolation to the physical (finite) \( b \) quark mass \( m_B \approx 4200 \) MeV by means of rather precise experimental results for \( c \) quarks, i.e. charm baryons.

<table>
<thead>
<tr>
<th>name</th>
<th>lattice</th>
<th>experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Lambda_b^0 )</td>
<td>429(30)</td>
<td>341(2)</td>
</tr>
<tr>
<td>( \Sigma_b )</td>
<td>629(28)</td>
<td>528(3)</td>
</tr>
<tr>
<td>( \Sigma^*_b )</td>
<td>651(28)</td>
<td>550(3)</td>
</tr>
<tr>
<td>( \Xi_b^- )</td>
<td>635(25)</td>
<td>513(3)</td>
</tr>
<tr>
<td>( \Omega_b^- )</td>
<td>877(27)</td>
<td>775(7)</td>
</tr>
</tbody>
</table>

- Differences between lattice and experimental results similar as for \( B/B_s \).

- In progress: continuum limit.

Forces between $B$ mesons (1)

- Goal: compute the potential of (or equivalently the force between) two $B$ mesons:
  - Treat the $b$ quark in the static approximation.
  - Consider only pseudoscalar mesons ($j^P = (1/2)^-$) and scalar mesons ($j^P = (1/2)^+$), which are among the lightest static-light mesons.
  - Study the dependence of the mesonic potential $V(R)$ on
    * the light quark flavor $u$ and/or $d$ (isospin),
    * the light quark spin (the static quark spin is irrelevant),
    * the type of the meson, i.e. $j^P = (1/2)^-$ or $j^P = (1/2)^+$.
Forces between $B$ mesons (2)

- Motivation/achievements:
  - First principles computation of a hadronic force, i.e. nuclear physics from elementary particles and their interactions.
  - For the first time with dynamical quarks (until now only quenched results).
  - For the first time also $j^P = (1/2)^+$ mesons (until now only $j^P = (1/2)^-$ mesons).

[M.W. [ETM Collaboration], PoS LATTICE2010, 162 (2010)]
Semileptonic decays $B \rightarrow D^{**}$ (1)

- The weak interactions change quark flavor, e.g. $b \rightarrow c + l + \nu$.
- Consider the specific weak decays

  $B \rightarrow D^{**} + l + \nu$.

  - $B$: $j = (1/2)^{-}$ $B$ meson.
  - $D^{**}$:
    * Orbitally excited $D$ meson (e.g. $\bar{c}u$) with parity $\mathcal{P} = +$.
    * Coupling of angular momentum $L = 1$ ("$P$ wave") and the light and the heavy quark spin yields four possible states:
      - Two $1/2$ $D^{**}$ ($L = 1$ and light quark spin $1/2$ are coupled to total angular momentum $j = 1/2$).
      - Two $3/2$ $D^{**}$ ($L = 1$ and light quark spin $1/2$ are coupled to total angular momentum $j = 3/2$).

  - $l + \nu$: lepton and corresponding neutrino.
Semileptonic decays $B \rightarrow D^{**}$ (2)

- There is a conflict between theory and experiment:
  - **Theory** (operator product expansion, sum rules):
    * Decay of $B$ to $3/2 \ D^{**}$ is more likely.
    * However:
      - Statements only hold in the limit $m_B \rightarrow \infty$.
      - Assumption: excited states can be neglected in sum rules.
      - Statements apply only for the “zero recoil situation”.
  - **Experiment**:
    * Decay of $B$ to $1/2 \ D^{**}$ is more likely.
    * However:
      - The measured signal for $1/2 \ D^{**}$ is extremely weak.
      - Assumption: no contributions of states “above $D^{**}$”.

→ Lattice computations can help, to resolve this conflict.
Semileptonic decays $B \rightarrow D^{**}$ (3)

- Computation of the decay probabilities:
  - Based on time-dependent perturbation theory (Fermi’s golden rule).
    * “Unperturbed” theory: QCD.
    * “Perturbing Hamiltonian”: weak interactions.
    * One has to compute the matrix elements
      $$\mathcal{M}_{fi} = \langle D^{**}_{1/2|3/2} l \nu | \mathcal{H}_{weak} | B \rangle.$$  
      - $\mathcal{M}_{fi}$ can be splitted into a leptonic part (contains $l$, $\nu$) and a hadronic part (contains $D^{**}_{1/2|3/2}$, $B$).
      - The leptonic part can be calculated analytically (“kinematical factors” in differential decay rates).
      - The hadronic part can be computed by means of lattice QCD (“Isgur-Wise functions” $\tau_{1/2}$ and $\tau_{3/2}$ in differential decay rates).
Semileptonic decays $B \rightarrow D^{**} (4)$

- Lattice result:

$$\tau_{1/2} = 0.30(3), \quad \tau_{3/2} = 0.53(2)$$

("$|\tau_{1/2}|^2$ is proportional to the decay probability in $1/2 D^{**}$"; ...).

[B. Blossier, M.W. and O. Pene [ETM Collaboration], JHEP 0906, 022 (2009)]

- Theory result (sum rules):

$$\left|\tau_{3/2}\right|^2 - \left|\tau_{1/2}\right|^2 \approx \frac{1}{4}$$

(comparison with the lattice result: $0.53^2 - 0.30^2 = 0.19 \approx 1/4$; sum rule fulfilled by around 80%).

- Experimental result (Belle):

$$\tau_{1/2} \approx 1.28, \quad \tau_{3/2} \approx 0.75.$$
Summary

- Lattice QCD is a method to compute QCD observables from first principles; systematic errors can be controlled and removed by suitable extrapolations.

- Lattice QCD is a powerful tool in the field of $B$ physics.

- Goals:
  - Precision computations followed by comparisons to experimental results ("search for new physics")
    $\rightarrow$ necessary accuracy for $B$ physics observables not yet reached.
  - Prediction/computation of observables, which are difficult/impossible to access experimentally
    $\rightarrow$ example: masses of excited $B$ mesons beyond $j = (3/2)^+$;
    $\rightarrow$ example: isospin, spin and parity dependent forces between $B$ mesons.
  - Qualitative understanding
    $\rightarrow$ example: level ordering of states, e.g. no reversal for $P_-$ and $P_+$;
    $\rightarrow$ example: decay of $B$ into $3/2$-$D^{**}$ more likely than into $1/2$-$D^{**}$.
Part 3: Further research interests and planned research.
Further research interests (1)

- During the past four years I roughly invested 1/3 of my research time for questions related to $B$ physics (the projects and results I have been reporting).

- Roughly another 1/3 went into a major project of the European Twisted Mass Collaboration concerned with simulations of QCD with 2+1+1 dynamical quark flavors (we are worldwide among the first to perform such simulations).
Further research interests (2)

- The remaining time I used for a variety of smaller projects:
  - **Determination of** $\Lambda_{\overline{\text{MS}}}$ **(establish contact between lattice QCD and perturbative QCD).**
  - **String breaking** in adjoint Yang-Mills theory and in QCD (theoretical aspects and numerical demonstration).
  - **Topology on the lattice, simulations at fixed topology** (preparatory steps for mixed action setups [overlap on twisted mass]).
  - (SU(2) four flavor) **QCD under extreme conditions** (finite temperature, strong external magnetic fields).
  - **Models based on topological excitations** for Yang-Mills theory/QCD both at zero temperature (merons, instantons, dimerons) and finite temperature (dyons) (qualitative understanding in particular regarding the phenomenon of confinement).
Planned research

- Continue ongoing projects, in particular ETMC simulations with 2+1+1 dynamical twisted mass quarks.

- Strange and charm meson spectroscopy (kaons, $D$ mesons, $D_s$ mesons, charmonium) with 2+1+1 dynamical twisted mass quarks.

- QCD at finite temperature (part of the Twisted Mass Finite Temperature Collaboration is located at the Johann Wolfgang Goethe University Frankfurt).

- QCD simulations at fixed topology, dependence of physical observables on the topological sector (relevant for mixed action setups including overlap quarks and for fully dynamical overlap simulations).

- ...

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some additional slides
Lattice QCD (A1)

- Numerical implementation of the path ...

  - Gluon field:
    * Action (in the continuum):
      \[
      S_{E,\text{gluons}} = \int d^4x \frac{1}{2g^2} \text{Tr}(F_{\mu\nu}F_{\mu\nu}).
      \]
    * To preserve gauge invariance, “indirect discretization” of the gluon field \( A_\mu \) via so-called gauge links (parallel transporters, which connect neighboring lattice sites):
      \[
      U_\mu(x) = P\left\{ \exp \left( -i \int_x^{x+ae_\mu} dz_\mu A_\mu(z) \right) \right\} \approx \exp \left( -ia A_\mu(x) \right).
      \]
    * Example: (no sum over \( \mu \) and \( \nu \)):
      \[
      a^4 \left( \text{Tr}(F_{\mu\nu}F_{\mu\nu}) + \mathcal{O}(a^2) \right) = \\
      = 6 \left( 1 - \frac{1}{3} \text{Re} \left( \text{Tr} \left( U_\mu(x)U_\nu(x+ae_\mu)U_\mu^\dagger(x+ae_\nu)U_\nu^\dagger(x) \right) \right) \right)
      \]
      (in electrodynamics this expression would be \( \propto (E_x)^2 \) or \( (B_x)^2 \) or ...).
\( b \) quarks with lattice QCD (A1)

- In contrast to light \( u, d \) and \( s \) quarks, heavy \( b \) quarks cannot be treated by means of the lattice techniques explained:
  - Field configurations close to classical solutions with small action are only weakly suppressed by \( e^{-S_E} \), i.e. play an important role in the path integral.
  - The classical equation of motion for quarks is the Dirac equation ("relativistic version of Schrödinger’s equation"):
    \[
    \left( \gamma_\mu (\partial_\mu - i A_\mu) + m_f \right) \psi^{(f)} = 0
    \]
    \( (\psi^{(f)} \) has four spin components; \( \gamma_\mu : 4 \times 4 \) matrices).
  - Solutions in the free case (\( A_\mu = 0 \)) are plane waves:
    \[
    \psi^{(f)}_{-s} = e^{-i(E(p)t - px)} u^s(p), \quad \psi^{(f)}_{+s} = e^{+i(E(p)t - px)} (u^s(p))^\dagger
    \]
    with \( E(p) = \sqrt{m_f^2 + p^2} \approx m_f \) for small momenta \( p \) and \( s = 1, 2 \), i.e. two solutions \( \psi^{(f)}_{-,s} \propto e^{-im_ft} \) and two solutions \( \psi^{(f)}_{+,s} \propto e^{+im_ft} \).

Marc Wagner, “Computation of \( B \) mesons and \( b \) baryons with lattice QCD”, January 20, 2011
**b quarks with lattice QCD (A2)**

- In contrast to light \( u, d \) and \( s \) quarks, heavy \( b \) quarks cannot be treated by means of the lattice techniques just explained:
  
  - Lattice representation of these solutions for \( b \) quarks:
    
    * \( m_b \approx 4000 \text{ MeV} \approx 20/\text{fm} \).
    * Typical lattice spacing: \( a = (1/10) \text{ fm} \).
    * Oscillations of the \( b \) quark field \( \psi_{\pm,s}^{(b)} \propto e^{\pm im_b t} \) cannot be resolved at typical present-day lattice spacings.
    * No such problems with light quarks (larger wave length of \( e^{\pm im_f t} \)).


**b quarks with lattice QCD (A3)**

- **Solution:** HQET (Heavy Quark Effective Theory).
  - Rewrite the $b$ quark field in terms of a new field according to
    
    $$
    \psi^{(b)} \rightarrow \psi'^{(b)} = e^{+im_bt}\psi^{(b)},
    $$
    
    i.e. perform a simple change of variables.
  - Two of the four solutions “loose” the strongly oscillating phase factor:
    $$
    \psi'_{-,s} \propto 1.
    $$
    - Two of the four solutions oscillate even stronger:
      $$
      \psi'_{+,s} \propto e^{-i2m_bt}.
      $$

    However, one can analytically perform the integration over field configurations corresponding to these strongly oscillating solutions.
  - Result: power series in $1/m_b$, where the leading order describes static ($=\text{infinitely heavy}$) $b$ quarks.

Marc Wagner, “Computation of $B$ mesons and $b$ baryons with lattice QCD”, January 20, 2011
Masses of $B$ and $B_s$ mesons (A1)

- Construction of a $B$ meson state:
  - The quark field operator $\psi^{(u)}(x)$ creates a $u$ quark at position $x$.
  - The quark field operator $\bar{\psi}^{(b)}(x)$ generates a $b$ antiquark at position $x$.
  - The following state contains a $B$ meson at position $x$:
    
    $$B^{(\Gamma)}|\Omega\rangle = \bar{\psi}^{(b)}(x)\Gamma\psi^{(u)}(x)|\Omega\rangle$$
    
    ($B^{(\Gamma)}$: meson creation operator).

  $\Gamma$: suitably chosen $4 \times 4$ matrix.
  - Acts on the spin indices of the quarks; realizes the desired angular momentum $J$ and/or $j$ as well as parity $P$.
  - A combination of the $\gamma$ matrices from the Dirac equation, e.g. $\Gamma = \gamma_5$ corresponds to $J^P = 0^-$ and $j^P = (1/2)^-$, the lightest $B$ meson.

  $B^{(\Gamma)}|\Omega\rangle$ is a superposition of $b$ meson states, which have the same quantum numbers $j^P$, but which differ in their radial quantum number.
Masses of $B$ and $B_S$ mesons (A2)

- Computation of the $B$ meson mass ($J = 0^-, j = (1/2)^-$):
  - Compute the vacuum expectation value
    \[
    C(t) = \langle \Omega | \left( \bar{\psi}^{(b)}(x, t) \gamma_5 \psi^{(u)}(x, t) \right)^\dagger \bar{\psi}^{(b)}(x, 0) \gamma_5 \psi^{(u)}(x, 0) | \Omega \rangle
    \]
    as a function of $t$ by means of lattice QCD.
  - $C(t)$: “meson correlation function”.

Marc Wagner, “Computation of $B$ mesons and $b$ baryons with lattice QCD”, January 20, 2011
Masses of $B$ and $B_S$ mesons (A3)

- Computation of the $B$ meson mass ($J = 0^-, j = (1/2)^-$):
  
  - Insert an identity in terms of energy eigenstates:
    
    $$C(t) = \langle \Omega | (B^{(\Gamma)}(t))^\dagger B^{(\Gamma)}(0) | \Omega \rangle = \ldots \approx_{t \gg 1} \text{const} \times e^{-m_B t}$$
    
    ($m_B$: mass of the $B$ meson; const: an irrelevant constant).
  
  - Extract $m_B$ e.g. by fitting $Ae^{-m_B t}$ to the computed points of $C(t)$ with $A$ and $m_B$ being the fit parameters.