



Bachelor Thesis

Tuning an anisotropic relativistic heavy quark action
in Quenched Lattice QCD
and computation of low-lying quarkonium states

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Abstract

In this bachelor thesis, I perform the tuning of an anisotropic relativistic heavy quark action (RHQ action) in quenched lattice QCD with three tunable parameters on a lattice with temporal extent $L_t = 64$, spatial extent $L_x = 24$ and inverse coupling $\beta = 5.9$. To this end, I calculate the mass m_{η_b} , the splitting $m_{\Upsilon(1S)} - m_{\eta_b}$ as well as the squared speed of light $c_{\eta_b}^2$ via the lattice dispersion relation for η_b . The three parameters of the action are iteratively improved to match these three observables on the lattice with their experimental values.

Zusammenfassung

In dieser Bachelorarbeit führe ich die Parameterabstimmung einer anisotropen relativistischen Schwerquark-Wirkung (RHQ-Wirkung) in gequenchter Gitter-QCD durch. Dabei werden die drei freien Parameter der Wirkung auf einem Gitter mit zeitlicher Ausdehnung $L_t = 64$, räumlicher Ausdehnung $L_x = 24$ und inverser Kopplungskonstante $\beta = 5.9$ iterativ so eingestellt, dass die aus der Simulation bestimmten Observablen m_{η_b} , $m_{\Upsilon(1S)} - m_{\eta_b}$ und $c_{\eta_b}^2$ mit ihren experimentellen Werten übereinstimmen.

Ehrenwörtliche Erklärung

Erklärung nach § 39 (15) Prüfungsordnung 2020 für den BAMA-Studiengang Physik

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1 Introduction

Quantum Chromodynamics (QCD) is the theory of quarks and gluons and their strong interactions. At scales of atomic nuclei ($10^{-15}\text{m} = 1\text{fm}$) and below it is typically the dominant force for describing hadrons. Mesons are hadrons described by QCD. They are bound states consisting of a quark and an antiquark $q\bar{q}'$. Meson spectra and other properties are studied both theoretically and experimentally [1], [2], [3].

Born-Oppenheimer effective field theory (BOEFT) is a possible approximation of QCD [4]. To appropriately tune its free parameters, its predictions have to be compared with reliable data either from experiments or from first principle lattice calculations. Of special interests are lattice predictions of highly excited as well as exotic mesonic states. This thesis aims to prepare a setup suitable for calculating properties of these states from first principle with lattice QCD.

Lattice QCD, in which all fields and operators are discretized on a finite lattice [5], introduces systematic errors into calculations such as finite volume effects and discretization errors.

To reduce the impact of discretization errors improved discretization of operators is desirable.

The relativistic heavy quark (RHQ) action used in this thesis contains such improvements [6]. It removes discretization errors of on-shell Green's function scaling of order $\mathcal{O}([m_0a]^n)$, $\mathcal{O}(|\vec{p}|a)$ and $\mathcal{O}(|\vec{p}a|[m_0a]^n)$ with $n = 1, 2, \dots$ [7]. The RHQ action contains three parameters that, for a specific lattice should be tuned nonperturbatively by comparing observables from the lattice with experimental observables. Once the action is tuned it can be used to calculate observables on the lattice.

This thesis is structured as follows.

In section 2 I define the path integral expectation value and the quenched approximation. I explain how to calculate smeared quark propagators. I describe the RHQ action and I explain how to calculate quarkonium correlators on the periodic lattice and derive its spectral decomposition.

I describe effective mass curves, and an algorithm with which the RHQ action can be tuned. I also explain how to extract the observables of the bottomonium system m_{η_b} , the spin averaged $m_{\Upsilon(1S)}$ and $c_{\eta_b}^2$ from the lattice data. I use these observables to tune the RHQ action.

In section 3 I describe, how I generate the quenched gauge field ensemble used in this thesis, and how I determined its lattice spacing. I explain the effects of fermionic Gauss smearing on the excited state contamination and I describe how its parameters were optimized in this thesis. I explain how I optimized the fit intervals for fits to the

quarkonium correlators.

Finally, I present the parameters and the values of the observables used for tuning, for all tuning steps and compare these observables with their experimental values.

In section 4 I present my conclusions on the used techniques and the obtained results. Finally, I give an outlook on follow-up work.

2 Theory

2.1 The quenched approximation

This section briefly reviews the path-integral formulation and the quenched approximation following [8]. Let $U_\mu(n)$ be the gauge fields, $\psi^{(f)}(n)$ be the quark field flavor f and let Λ be the set of all lattice sites. Let S_G denote the gauge action and let S_F be the fermion action. The Euclidean path integral expectation value of an observable $\mathcal{A}$ is defined as

$$\langle \mathcal{A} \rangle := \frac{1}{Z} \int D[\psi, \bar{\psi}] D[U] \exp(-S_F[\psi, \bar{\psi}, U] - S_G[U]) \mathcal{A}[\psi, \bar{\psi}, U] \quad (1)$$

where the partition function Z is defined as

$$Z := \int D[\psi, \bar{\psi}] D[U] \exp(-S_F[\psi, \bar{\psi}, U] - S_G[U]) \quad (2)$$

and the integrations measures are defined as:

$$D[U] := \prod_{n \in \Lambda} \prod_{\mu=1}^4 dU_\mu(n) \quad (3)$$

$$D[\psi, \bar{\psi}] := \prod_{n \in \Lambda} \prod_{f, \alpha, c} d\psi^{(f)}(n)_\alpha d\bar{\psi}^{(f)}(n)_\alpha. \quad (4)$$

$\langle \mathcal{A} \rangle$ can be split into the fermionic expectation value $\langle \mathcal{A} \rangle_F$ and the gauge field expectation value $\langle \mathcal{B} \rangle_G$ defined by:

$$\langle \mathcal{A} \rangle_F[U] := \frac{1}{Z_F[U]} \int D[\psi, \bar{\psi}] \exp(-S_F[\psi, \bar{\psi}, U]) \mathcal{A}[\psi, \bar{\psi}, U] \quad (5)$$

$$Z_F[U] := \int D[\psi, \bar{\psi}] \exp(-S_F[\psi, \bar{\psi}, U]) \quad (6)$$

$$\langle \mathcal{B} \rangle_G := \frac{1}{Z} \int D[U] \exp(-S_G[U]) \mathcal{B}[U] Z_F[U] \quad (7)$$

$Z_F[U]$ is called the fermionic determinant. Notice that $\langle \mathcal{A} \rangle = \langle \langle \mathcal{A} \rangle_F \rangle_G$. For a numerical evaluation of equation (1) one can use importance sampling, and write

$$\langle \mathcal{A} \rangle = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \langle \mathcal{A} \rangle_F[U_n]. \quad (8)$$

where the U_n are chosen according to the probability distribution density:

$$dP(U) = \frac{D[U] \exp(-S_G[U]) Z_F[U]}{\int D[U] \exp(-S_G[U]) Z_F[U]}. \quad (9)$$

The quenched approximation is defined by setting $Z_F[U] = 1$ in equation (9). In this thesis I use the quenched approximation. At finite statistics the path integral expectation value in the quenched approximation $\langle \mathcal{A} \rangle_{\text{quenched}}$ can be approximated as:

$$\langle \mathcal{A} \rangle_{\text{quenched}} \approx \frac{1}{N} \sum_{n=1}^N \langle \mathcal{A} \rangle_F[U_n]. \quad (10)$$

where the U_n are chosen according to the probability distribution density:

$$dP'(U) = \frac{D[U] \exp(-S_G[U])}{\int D[U] \exp(-S_G[U])}. \quad (11)$$

2.2 Action

In this thesis, I use the clover-improved anisotropic relativistic heavy-quark action (12) given in [7].

$$S_Q(m_0, \nu, c_{sw}) = a^4 \sum_{n,m} \bar{\psi}(m) D_{\text{RHQ}}(m|n) \psi(n) \quad (12)$$

Here

$$D_{\text{RHQ}}(m|n) := \left(m_0 + \gamma_4 D_4 + \nu \gamma_i D_i - \frac{a}{2} (D_4)^2 - \frac{a}{2} \nu (D_i D_i) + \sum_{\mu, \nu} \frac{ia}{4} c_{sw} \sigma_{\mu\nu} F_{\mu\nu} \right)_{mn}. \quad (13)$$

Here m_0 is the bare quark mass for the quark of flavor Q, ν is the anisotropy parameter and c_{sw} is the Sheikholeslami-Wohlert coefficient. The discretizations of the first and the second partial derivatives, as well as the discretizations of the Yang-Mills field

strength tensor $F_{\mu\nu}$ are given as:

$$(14)$$

$$D_\mu \psi(n) = \frac{1}{2a} \left[U_\mu(n) \psi(n + \hat{\mu}) - U_\mu^\dagger(n - \hat{\mu}) \psi(n - \hat{\mu}) \right] \quad (15)$$

$$D_\mu^2 \psi(n) = \frac{1}{a^2} \left[U_\mu(n) \psi(n + \hat{\mu}) + U_\mu^\dagger(n - \hat{\mu}) \psi(n - \hat{\mu}) - 2\psi(n) \right] \quad (16)$$

$$F_{\mu\nu} \psi(n) = \frac{1}{8a^2} \sum_{s,s'=\pm 1} ss' \left[U_{s\mu}(n) U_{s'\nu}(n + s\hat{\mu}) U_{s\mu}^\dagger(n + s'\hat{\nu}) U_{s'\nu}^\dagger(n) - \text{h.c.} \right]. \quad (17)$$

$\sigma_{\mu\nu}$ and $U_{-\mu}$ are defined as:

$$\sigma_{\mu\nu} := \frac{i}{2} [\gamma_\mu, \gamma_\nu] \quad (18)$$

$$U_{-\mu}(n) := U_\mu(n - \hat{\mu})^\dagger. \quad (19)$$

According to [7] the parameters can be tuned to remove discretization errors of order $\mathcal{O}(|\vec{p}|a)$, $\mathcal{O}(|\vec{p}|a(m_0a)^n)$ and $\mathcal{O}((m_0a)^n)$ for $n = 1, 2, \dots$ for on-shell greens functions, where $|\vec{p}|$ and m_0 are given in physical units.

The tuned RQH action (12) can then be used to describe quarks with $m_0a < 1$. Note that D_{RQH} satisfies equation (41), as I show in section 5.4. In the following I exclusively consider this action.

2.3 Propagators

This section briefly reviews propagators and fermionic smearing following [8].

The propagator $D^{(Q)-1}(n|m)_{\beta\alpha}$ from a source position m to a sink position n is the inverse of the Dirac operator $D^{(Q)}(n|m)_{\beta\alpha}$. It satisfies

$$\sum_{\alpha,a,m} D^{(Q)}(n|m)_{\beta\alpha} D^{(Q)-1}(m|l)_{\alpha\gamma} = \delta_{n,l} \delta_{\beta\gamma} \delta_{bc}. \quad (20)$$

The label Q stands for the quark flavor, the indices α and β denote spin indices and a and b denote color indices.

For a fixed color index a_0 , a fixed spin index α_0 and a fixed lattice site m_0 a point source $S_0^{(m_0,\alpha_0,a_0)}(m)_\alpha$ is defined as:

$$S_0^{(m_0,\alpha_0,a_0)}(m)_\alpha := \delta_{m,m_0} \delta_{\alpha,\alpha_0} \delta_{a,a_0}. \quad (21)$$

A point to all propagator is defined as the action of the propagator on a point source:

$$D^{(Q)-1}(n|m_0)_{\beta\alpha_0} = \sum_{m,\alpha,a} D^{(Q)-1}(n|m)_{\beta\alpha} S_0^{(m_0,\alpha_0,a_0)}(m)_a^\alpha. \quad (22)$$

One can replace the point source in equation (22) by a smeared source $S^{(m_0,\alpha_0,a_0)}(m)_a^\alpha$ resulting in the smeared point to all propagator

$$D_S^{(Q)-1}(n|m_0)_{\beta\alpha_0} = \sum_{m,\alpha,a} D^{(Q)-1}(n|m)_{\beta\alpha} S^{(m_0,\alpha_0,a_0)}(m)_a^\alpha. \quad (23)$$

Such smearing can help reduce excite state contamination described in section 2.5. A commonly used approximation to Gaussian smearing is given by the kernel $G^{(N_{\text{smear}})}$ [7]. Its action on a source field S is defined by equations (24) and (25).

$$G^{(N_{\text{smear}})} := \left(1 + \frac{\sigma_{\text{smear}}^2}{4N_{\text{smear}}} \Delta\right)^{N_{\text{smear}}} \quad (24)$$

$$\Delta S(n) = \sum_{k=1}^3 \left(U_k(n) S(n + \hat{k}) + U_k^\dagger(n - \hat{k}) S(n - \hat{k}) - 2S(n) \right) \quad (25)$$

N_{smear} is the number of smearing steps and σ_{smear} is the smearing radius. A possible smeared point source is therefore

$$S^{(m_0,\alpha_0,a_0)} = G^{(N_{\text{smear}})} S_0^{(m_0,\alpha_0,a_0)}. \quad (26)$$

To calculate the smeared point to all propagator defined in equation (23) which I abbreviate with ϕ one can solve the system of equations:

$$D\phi = S. \quad (27)$$

A modern method to solve this set of equations is with variations of gradient (CG) algorithm described in [8]. Such methods will not be discussed here.

2.4 Quarkonium Correlators

Let $\mathcal{O}_Q$ be a single quarkonium operator of the form

$$\mathcal{O}_Q = \bar{Q} \Gamma Q. \quad (28)$$

Here Q is a spinor of flavor Q and Γ is some monomial in the Euclidean γ -matrices, acting in spin space. Depending on the choice of Γ $\mathcal{O}_Q$ has different quantum numbers. Table 1 shows low-lying quarkonium states, as well as Γ that creates states with the corresponding quantum numbers and the experimental masses taken from the Particle Data Group (PDG) [2].

Table 1: Low-lying bottomonium states, quantum numbers, interpolating operators, and PDG masses.

State	J^{PC}	Γ structure	Mass [MeV]
$\eta_b(1S)$	0^{-+}	γ_5	9398.7 ± 2.0
$\Upsilon(1S)$	1^{--}	γ_i	9460.30 ± 0.26
$\chi_{b0}(1P)$	0^{++}	$\mathbf{1}$	9859.44 ± 0.42
$\chi_{b1}(1P)$	1^{++}	$\gamma_i \gamma_5$	9892.78 ± 0.40

Here γ_μ are the Euclidean gamma matrices that satisfy

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}, \quad \gamma_\mu^\dagger = \gamma_\mu, \quad (29)$$

for $\mu = 1, 2, 3, 4$ and the hermitian γ_5 is defined by

$$\gamma_5 := \gamma_1 \gamma_2 \gamma_3 \gamma_4. \quad (30)$$

2.4.1 Position space correlators

On the lattice the single quarkonium creation operator $\mathcal{O}_Q$ has to be given in position space. For that I set

$$\mathcal{O}_Q(n) = \bar{Q}(n) \Gamma Q(n). \quad (31)$$

The correlator in position space on a single gauge field configuration $G(n - m)$ can be defined as

$$G(n - m) := \langle \mathcal{O}_Q(n) \bar{\mathcal{O}}_Q(m) \rangle_F \quad (32)$$

I need the identity

$$\gamma_4 \Gamma^\dagger \gamma_4 = \eta_\Gamma \Gamma \quad (33)$$

where $\eta_\Gamma = \pm 1$, which holds if Γ is a monomial in the Euclidean γ -matrices.

$$\bar{\mathcal{O}}_Q(m) = \mathcal{O}_Q^\dagger(m) = -Q(m)^\dagger \gamma_4^2 \Gamma^\dagger (\bar{Q}(m))^\dagger = -\bar{Q}(m) \gamma_4 \Gamma^\dagger \gamma_4 Q^\dagger(n) = -\eta_\Gamma \bar{Q}(m) \Gamma Q(m) \quad (34)$$

For the second equality sign, I used $\gamma_4^2 = 1$, equation (31) and the Grassmann property of the quark fields.

I used $\bar{Q} = Q^\dagger \gamma_4$ for the third and equation (33) for the last equality sign. I continue to calculate

$$G(n-m) = \langle \mathcal{O}_Q(n) \bar{\mathcal{O}}_Q(m) \rangle_F \quad (35)$$

$$= -\eta_\Gamma \left\langle \bar{Q}(n)_{a_1}^{\alpha_1} \Gamma_{\alpha_1 \alpha_2} Q(n)_{a_1}^{\alpha_2} \bar{Q}(m)_{b_1}^{\beta_1} \Gamma_{\beta_1 \beta_2} Q(m)_{b_1}^{\beta_2} \right\rangle_F \quad (36)$$

$$= -\eta_\Gamma \Gamma_{\alpha_1 \alpha_2} \Gamma_{\beta_1 \beta_2} \left\langle \bar{Q}(n)_{a_1}^{\alpha_1} Q(n)_{a_1}^{\alpha_2} \bar{Q}(m)_{b_1}^{\beta_1} Q(m)_{b_1}^{\beta_2} \right\rangle_F. \quad (37)$$

For the second equality sign I use equations (31) and (34) and write the expression out in index notation. α_i and β_i denote spin indices while a_i and b_i denote color indices.

$$\begin{aligned} &= -\eta_\Gamma \Gamma_{\alpha_1 \alpha_2} \Gamma_{\beta_1 \beta_2} \times \\ &\left(\left\langle Q(n)_{a_1}^{\alpha_2} \bar{Q}(n)_{a_1}^{\alpha_1} \right\rangle_F \left\langle Q(m)_{b_1}^{\beta_2} \bar{Q}(m)_{b_1}^{\beta_1} \right\rangle_F - \left\langle Q(m)_{b_1}^{\beta_2} \bar{Q}(n)_{a_1}^{\alpha_1} \right\rangle_F \left\langle Q(n)_{a_1}^{\alpha_2} \bar{Q}(m)_{b_1}^{\beta_1} \right\rangle_F \right) \end{aligned} \quad (38)$$

$$\begin{aligned} &= -\eta_\Gamma \Gamma_{\alpha_1 \alpha_2} \Gamma_{\beta_1 \beta_2} \times \\ &\left(D^{(Q)-1}(n|n)_{a_1 a_1}^{\alpha_2 \alpha_1} D^{(Q)-1}(m|m)_{b_1 b_1}^{\beta_2 \beta_1} - D^{(Q)-1}(m|n)_{b_1 a_1}^{\beta_2 \alpha_1} D^{(Q)-1}(n|m)_{a_1 b_1}^{\alpha_2 \beta_1} \right) \end{aligned} \quad (39)$$

$$\begin{aligned} &= -\eta_\Gamma \text{Tr}\{D^{(Q)-1}(n|n)\Gamma\} \text{Tr}\{D^{(Q)-1}(m|m)\Gamma\} \\ &+ \eta_\Gamma \text{Tr}\{D^{(Q)-1}(m|n)\Gamma D^{(Q)-1}(n|m)\Gamma\} \end{aligned} \quad (40)$$

First I use Wick's theorem. For the third equality sign, I use the Trace in both spin and color space Tr . I have also introduced the propagator $D^{(Q)-1}(m|n)$ from the source position m to the sink position n .

Another common property of Dirac operators is γ_5 hermiticity, e.g. the following equation holds.

$$D^\dagger = \gamma_5 D \gamma_5 \quad (41)$$

If this holds, then also the propagator is γ_5 hermitian. In this thesis, the action used is defined in section 2.2, and the proof for the γ_5 hermiticity of this action can be found in section 5.4. If I assume γ_5 hermiticity, I find

$$\begin{aligned} &\langle \mathcal{O}(n) \bar{\mathcal{O}}(m) \rangle_F = \\ &- \eta_\Gamma \text{Tr}\{D^{(Q)-1}(n|n)\Gamma\} \text{Tr}\{D^{(Q)-1}(m|m)\Gamma\} \\ &+ \eta_\Gamma \text{Tr}\{\gamma_5 (D^{(Q)-1}(n|m))^\dagger \gamma_5 \Gamma D^{(Q)-1}(n|m)\Gamma\}. \end{aligned} \quad (42)$$

Here the dagger on the second to last inverse Dirac operator acts on spin and color indices.

The term containing inverse Dirac operators connecting sites to themselves, is called a disconnected term.

In this thesis, disconnected terms are not calculated.

2.4.2 Momentum space correlators

The single quarkonium interpolating operator at definite spatial momentum $\vec{p}$ $\tilde{\mathcal{O}}_Q(\vec{p}, t)$ is defined as the Fourier-transformed of the position space quarkonium interpolating operator.

$$\tilde{\mathcal{O}}_Q(\vec{p}, t) = \frac{1}{\sqrt{|\Lambda_3|}} \sum_{\vec{n}} e^{-i\vec{p}\vec{n}} \mathcal{O}_Q(\vec{n}, t) \quad (43)$$

$|\Lambda_3|$ is the number of points $\vec{n}$ can take. An important object is the correlator at definite spatial momentum $\vec{p}$ $C(\vec{p}, t)$ which is defined as:

$$C(\vec{p}, t) := \left\langle \tilde{\mathcal{O}}_Q(\vec{p}, t + t') \bar{\tilde{\mathcal{O}}}_Q(\vec{p}, t') \right\rangle = \quad (44)$$

$$\left(\frac{1}{\sqrt{|\Lambda_3|}} \right)^2 \sum_{\vec{n}, \vec{m}} e^{-i(\vec{p}\vec{n} - \vec{p}\vec{m})} \left\langle \mathcal{O}_Q(\vec{n}, t + t') \bar{\mathcal{O}}_Q(\vec{m}, t') \right\rangle = \quad (45)$$

$$\frac{1}{|\Lambda_3|} \sum_{\vec{n}, \vec{m}} e^{-i\vec{p}(\vec{n} - \vec{m})} \langle G(\vec{n} - \vec{m}, t) \rangle_G \quad (46)$$

I first used Equation (43) and translational invariance to rewrite $G(\vec{n} - \vec{m}, t) = \langle \mathcal{O}_Q(\vec{n}, t + t') \bar{\mathcal{O}}_Q(\vec{m}, t') \rangle_F$ where $G(n - m)$ is defined in equation (32).

$$C(\vec{p}, t) = \frac{1}{|\Lambda_3|} \sum_{\vec{n}, \vec{r}} e^{-i(\vec{p}\vec{r})} \langle G(\vec{r}, t) \rangle_G \quad (47)$$

$$= \sum_{\vec{r}} e^{-i\vec{p}\vec{r}} \langle G(\vec{r}, t) \rangle_G \quad (48)$$

I first reindexed the sum over m with the shift $\vec{n} - \vec{m} = \vec{r}$, and then I collapsed $\sum_n = |\Lambda_3|$. By substituting $G(r, t)$ back and reverting the index shift I calculate

$$C(\vec{p}, t) = e^{+i\vec{p}\vec{m}} \sum_{\vec{n}} e^{-i\vec{p}\vec{n}} \left\langle \mathcal{O}_Q(\vec{n}, t + t') \bar{\mathcal{O}}_Q(\vec{m}, t') \right\rangle. \quad (49)$$

In this form it is evident, that a knowledge of the lhs. of equation (49) for any fixed source point $(\vec{m}, t')$ is sufficient to compute the rhs. However, at finite statistics better

results can be achieved by averaging over multiple source points.

$$C(\vec{p}, t) = \left\langle \frac{1}{\#S_{\text{scr}}} \sum_{(\vec{m}, t') \in S_{\text{scr}}} \tilde{\mathcal{O}}_Q(\vec{p}, t + t') \bar{\mathcal{O}}_Q(\vec{m}, t') e^{i\vec{p}\vec{m}} \right\rangle \quad (50)$$

Since energies according to the continuum dispersion relation

$$E(\vec{p}) = \sqrt{m^2 + \vec{p}^2} \quad (51)$$

only depend on $p = |\vec{p}|$ statistics can be further improved by only considering the absolute value of the momentum. I define $C(p, t)$ the average correlator of a momentum shell as:

$$C(p, t) := \frac{1}{N_p} \sum_{|\vec{p}|=p} C(\vec{p}, t). \quad (52)$$

Here N_p is the number of momenta with $|\vec{p}| = p$ that can be realized on the lattice. For $\vec{p} = \vec{0}$ I define:

$$C(t) := C(\vec{0}, t). \quad (53)$$

In section 5.2 I show, that if only contributions from the vacuum are considered $C(\vec{p}, t)$ on the periodic lattice can be approximated as:

$$C(\vec{p}, t) \approx \frac{2}{Z} \sum_s A_{\Omega s}(\vec{p}) e^{-\frac{\beta}{2}(E_s(\vec{p}) + E_\Omega)} \cosh \left[(E_s(\vec{p}) - E_\Omega) \left(t - \frac{\beta}{2} \right) \right]. \quad (54)$$

Here $A_{\Omega s}(\vec{p})$ is an overlap factor defined by:

$$A_{\Omega s}(\vec{p}) := \langle \vec{0}, s_\Omega | \tilde{\mathcal{O}}_Q(\vec{p}) | \vec{p}, s \rangle \langle \vec{p}, s | \tilde{\mathcal{O}}_Q^\dagger(\vec{p}) | \vec{0}, s_\Omega \rangle. \quad (55)$$

Sufficiently far away from the boundaries $t = N_T$ and $t = 0$ the ground state labeled by $s = 0$ dominates and I write

$$C(\vec{p}, t) \approx \frac{2}{Z} A_{\Omega 0}(\vec{p}) e^{-\frac{\beta}{2}(E_0(\vec{p}) + E_\Omega)} \cosh \left[(E_0(\vec{p}) - E_\Omega) \left(t - \frac{\beta}{2} \right) \right]. \quad (56)$$

With the definition $A_{\Omega s}(p) := \frac{1}{N_p} \sum_{|\vec{p}|=p} A_{\Omega s}(\vec{p})$ and $E_s(p) := \frac{1}{N_p} \sum_{|\vec{p}|=p} E_s(\vec{p})$ and equation (52) I calculate

$$C(p, t) \approx \frac{2}{Z} A_{\Omega 0}(p) e^{-\frac{\beta}{2}(E_0(p) + E_\Omega)} \cosh \left[(E_0(p) - E_\Omega) \left(t - \frac{\beta}{2} \right) \right]. \quad (57)$$

2.5 Effective mass

Let $C(t)$ be a correlator at definite spatial momentum $\vec{p} = \vec{0}$ as described in section 2.4. The leading-order contribution to $C(t)$ for quarkonium is of the form $2A \cosh(m(t - \beta/2))e^{-m\frac{\beta}{2}}$, if t is far away from the boundaries $t = 0$ and $t = N_T$.

Here m is the mass of the state, $\beta = N_T$ is the number of lattice points in the temporal direction, and A is a positive real number.

The effects of the subleading terms are called excited-state contaminations. To keep them at a minimum one can choose an interval for subsequent analysis, such that the contributions of excited-states in that interval are negligible. One standard test for this is to define an effective mass, a measure of the mass m , that only uses neighboring time points.

In this thesis, I use the cosh effective mass $m_{\text{eff}}(t)$

$$m_{\text{eff}}(t) = \text{arcosh} \left(\frac{C(t+1) + C(t-1)}{2C(t)} \right) \quad (58)$$

In the limit in which the subleading terms become zero $m_{\text{eff}}(t)$ becomes constant. Once an interval has been found where the excited-state contamination is sufficiently small, all subsequent analysis will be conducted on this interval only.

Note that the leading-order contribution to $C(t)$ is symmetric around the point $t = N_T/2$. At finite statistics, better results can be achieved by averaging the forward and the backward parts of the correlator before using equation (58). This was done in this thesis.

2.6 Tuning

The RHQ-action $S_Q(m_0, \nu, c_{sw})$ from subsection 2.2 can be used to describe heavy quarks. For this the parameters of the action have to be chosen, such that lattice results match the experimental data, up to finite volume effects and discretization errors.

I set $P = (m_0, \nu, c_{sw})$ and call the optimal parameters P_{opt} , which can be determined non perturbatively on the lattice.

For that, let $O_i^{\text{lat}}, O_i^{\text{exp}}, i = 1, 2, 3$ be the same observables on the lattice, and in the experiment respectively. O_i^{lat} are functions of the parameters P . This corresponds to finding the roots of $F(P)$ with $F_i(P) := O_i^{\text{exp}} - O_i^{\text{lat}}(P)$.

If an initial guess $P^{(0)}$ for the location of the root is known, such that F is locally well described by a non-constant affine linear function, then Newton-Raphson is an iterative root finding algorithm.

Let $J(P)$ be the Jacobian matrix of F at P such that $J_{ij}(P) = \frac{\partial F_i}{\partial P_j}$ and let $P^{(n)}$ be the n -th guess for P then $P^{(n+1)} = P^{(n)} - J^{-1}(P^{(n)}) F(P^{(n)})$. If the Jacobian is not known analytically, it can be numerically estimated, by discretizing the derivatives according to $\frac{\partial F_i}{\partial P_j} \rightarrow \frac{F_i(P^{(n)} + h_j \hat{e}_j) - F_i(P^{(n)} - h_j \hat{e}_j)}{2h_j}$. h_j is a positive small number.

This was done by the authors of [7]. They propose to stop the tuning process, if

$$P_j^{(n)} - h_j \leq P_j^{(n+1)} \leq P_j^{(n)} + h_j \quad (59)$$

holds.

This corresponds to the requirement, that the last tuning step is an interpolation rather than an extrapolation. $P^{(n+1)}$ are then considered to be the tuned parameters P^{tuned} of the action.

In this thesis, I follow the approach of [7], but I also consider that O_i^{lat} has a statistical error.

To do this, I use the methods described in the subsection 5.1 to calculate the jackknife estimate of $P^{(n+1)}$ with its jackknife error, which I call $\sigma_P = (\sigma_{m_0}, \sigma_\nu, \sigma_{c_{sw}})^T$.

σ_P should be compared to the change in parameters $P_i^{(n+1)} - P_i^{(n)}$.

If $\frac{(\sigma_P)_i}{P_i^{(n+1)} - P_i^{(n)}}$ is much larger than one for all $i = 1, 2, 3$, no meaningful improvement should be expected.

In particular, if the h_i are chosen to be very small the jackknife estimates of $J(P^{(n)})$ may become dominated by noise, and as a result may be ill conditioned. In such a case the jackknife mean could be dominated by noise, and the Newton-Raphson algorithm may not converge.

Each h_j has to be chosen small enough, such that O_i^{exp} equals $O_i^{\text{lat}}(P)$ up to desired precision for $i = 1, 2, 3$.

In this thesis, I use the mass of η_b $O_1^{\text{exp}} = m_{\eta_b}$ the splitting $O_2^{\text{exp}} = m_{\Upsilon(1S)} - m_{\eta_b}$ where $m_{\Upsilon(1S)}$ is the spin averaged mass of $\Upsilon(1S)$ and $O_3^{\text{exp}} = c_{\eta_b}^2$ as observables. These are well known experimentally and are sensitive to change P .

I perform a χ^2 minimizing fit of $C(p, t)$ calculated with equations (52) and (50) for η_b to equation (57) to extract the dispersion relation $(E_{0, \eta_b}(p) - E_\Omega)$ for η_b . $m_{\eta_b} = (E_{0, \eta_b}(0) - E_\Omega)$ follows.

To extract the $c_{\eta_b}^2$, I perform a further correlated fit to the dispersion relation

$$E_{0,\eta_b}(p) - E_\Omega = \sqrt{m_{\eta_b}^2 + p^2 c_{\eta_b}^2} \quad (60)$$

equivalent to equation (51), where masses and energies are given in MeV/c².

The mass $m_{\Upsilon(1S)}$ of the spin averaged $\Upsilon(1S)$ is extracted in the same manner as for η_b .

3 Results

3.1 Generating and analyzing quenched gauge field configurations

Unless stated otherwise, all quantities are given in lattice units. For generating quenched gauge field configurations, I chose a lattice with spatial extent $L_X = 24$ and with temporal extent $L_T = 64$. As inverse coupling strength I chose $\beta = 5.9$. In total, I generated 2000 gauge field configurations.

According to [9] equation (61) is a parametrization for $\ln(a(\beta)/r_0)$ for $5.7 \leq \beta \leq 6.57$ with relative statistical uncertainty $\frac{\Delta a}{a}(\beta)$ as parametrized by equation (62). Here $r_0 = 0.5\text{fm}$ is the hadronic scale or Sommer scale introduced in [10].

$$\ln(a/r_0) = -1.6805 - 1.7139(\beta - 6) + 0.8155(\beta - 6)^2 - 0.6667(\beta - 6)^3 \quad (61)$$

$$\frac{\Delta a}{a}(\beta) = 0.3\% + \frac{0.6\% - 0.3\%}{6.57 - 5.7}(\beta - 5.7) \quad (62)$$

Using this I obtained a lattice spacing of $a(5.9) = (0.11153 \pm 0.00041)\text{fm}$.

It should be noted, that this precision is misleadingly high, as it does not contain the systematic error of estimating the lattice spacing with the static force.

Grid Python Toolkit (GPT) [11] is a Python library with C++ backend, used throughout this thesis. GPT is based on Grid [12].

I used the $SU(2)$ -heatbath algorithm provided by the GPT library to generate quenched gauge field configurations. To study thermalization, I used GPT to compute the average plaquette P , for every saved configuration. P is defined by:

$$P := \frac{1}{6|\Lambda|N_c} \sum_{n \in \Lambda} \sum_{\mu < \nu} \text{Re Tr}(U_{\mu\nu}(n)), \quad (63)$$

$$U_{\mu\nu}(n) := U_\mu(n)U_\nu(n + \hat{\mu})U_\mu(n + \hat{\nu})^\dagger U_\nu(n)^\dagger. \quad (64)$$

Here N_c is the number of color. To reduce the impact of statistical fluctuations, I computed a running average over the plaquette which I defined as follows. Let $\text{plaq}(i)$ be the average plaquette P of the i -th configuration, let N_{av} be the number of

configurations to average over. The running average over N_{av} configurations $\text{plaq}_{\text{av}}(i)$ I defined as:

$$\text{plaq}_{\text{av}}(i) := \frac{1}{N_{\text{av}}} \sum_{j=0}^{N_{\text{av}}-1} \text{plaq}(i-j). \quad (65)$$

I note that this quantity is not defined if $i < N_{\text{av}}$, and that thermalizes up to $N_{\text{av}} - 1$ configurations later than the plaquette.

In the top plot of figure 1 I show plaq_{av} for $N_{\text{av}} = 50$ and configuration numbers 50 – 2000.

From the left, up until approximately configuration number 200 the plaquette has a clear downwards trend. Further to the right, it seems to thermalize. To set a point, where the plaquette thermalizes with higher precision, I inspected a smaller interval, and plot the average plaquette. The bottom plot of figure 1 shows plaq for configuration numbers 50 – 600. At around the 200-th configuration the downward trend stops. In order to guarantee, that I did not use a configuration before thermalization for subsequent analyses I conservatively choose $N_{\text{therm}} = 250$.

3.2 Optimizing fermionic smearing

The excited state contamination discussed in subsection 2.5 can be reduced by means of fermionic smearing described in section 2.3. I used the GPT library for the numerical implementation of equation (27) and (23). In this thesis I used Gaussian smearing described in section 2.3 and I chose $\sigma_{\text{smear}} = 1$ and optimize N_{smear} . For this I used the parameters of the 0-th tuning step which can be found in table 5 to calculate the correlator at zero spatial momentum $C(t)$ as described in section 2.4. The effective mass m_{eff} was calculated using equation (58). For these calculations, I used 100 different gauge field configurations, with 5 source points each.

I repeated the calculation for $N_{\text{smear}} = 1, 2, 3, 4$, and plotted the effective mass curves in the two plots in figure 2.

In the top plot I show m_{eff} as a function of t for $N_{\text{smear}} = 1, 2, 3, 4$, for $t \geq 5$. For low values of t , $N_{\text{smear}} = 1$ clearly leads to the highest effective mass values and thus the highest excited state contamination.

The bottom plot shows the same data as the top plot, excluding $N_{\text{smear}} = 1$.

There one can see that $N_{\text{smear}} = 2$ seems to generate the lowest effective mass curves for early time slices, of all tested values of N_{smear} . The difference is not significant. I chose $N_{\text{smear}} = 2$ for all further calculations.

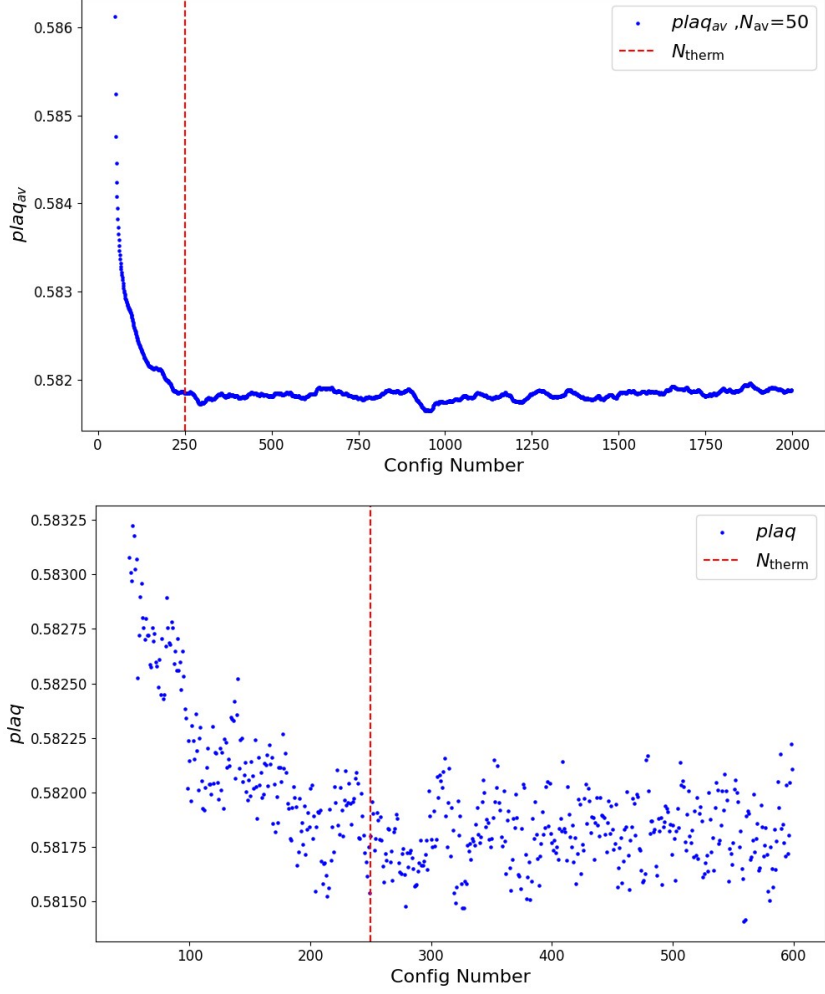


Figure 1: Top: $plaq_{av}$ with $N_{av} = 50$, Bottom: $plaq$

3.3 Interval setting

For the tuning described in subsections 2.6 and 3.4 fits to $C(p, t)$ have to be done. The interval in which these fits are taken should on the one hand have low excited state contamination, on the other hand one would expect fits there to have a reduced χ^2_{red} near one.

Figure 3 shows the effective mass for the parameters of the zeroth tuning step. The plateau begins at approximately $t_{min} = 15$ and ends at approximately $t_{max} = 26$.

I varied the bounds of this plateau and for each of these I calculate the mean value over all momentum shells of $|1 - \chi^2_{red}|$ for the fits to equation (57). Since $\chi^2_{red} \approx 1$ indicates data compatible with the model function, this is indicative of how strong effects of excited state contamination affect fits to correlators. In table 2 I report these results. The lowest value is achieved with $t_{min} = 15$ and $t_{max} = 26$. In all further

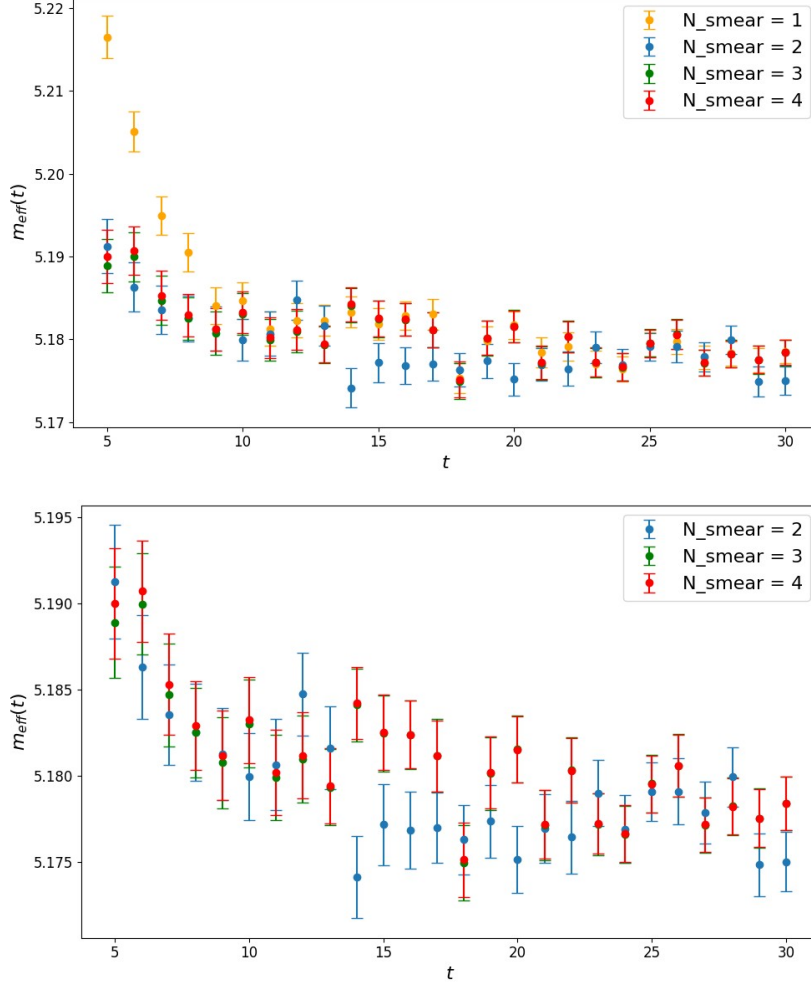


Figure 2: Effective masses m_{eff} for η_b . Top: $N_{\text{smear}} = 1, 2, 3, 4$, $t \geq 5$. Bottom: $N_{\text{smear}} = 2, 3, 4$, $15 \leq t \leq 26$.

analyses this is the fit interval I chose.

Table 2: Mean over all momentum shells of $|1 - \chi_{\text{red}}^2|$ for fit of $C(p, t)$ to equation (57).

$t_{\text{min}}/a \backslash t_{\text{max}}/a$	24	25	26	27
14	0.62	0.58	0.40	0.56
15	0.078	0.077	0.043	0.33
16	0.20	0.14	0.082	0.45

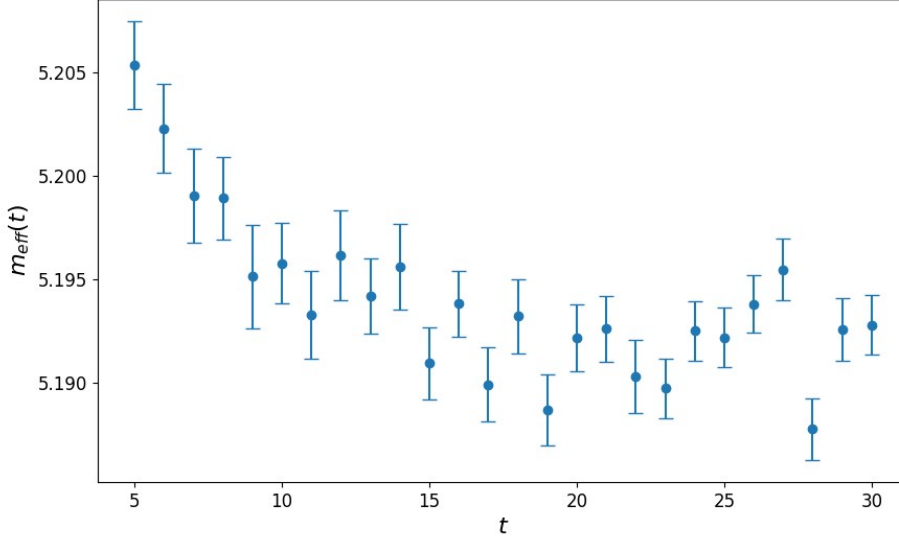


Figure 3: Shows m_{eff} for $t \geq 5$.

3.4 Tuning

In [13] the RHQ action was tuned with the heavy-strange mesons B_s , $B_s^{(*)}$, D_s and $D_s^{(*)}$.

In [13] they perform the tuning for an ensemble labeled with C005 and give a lattice spacing of $a \approx 0.111\text{fm}$. Their lattice geometry is $24^3 \times 64$ with 311 gauge field configurations.

The ensemble used in this thesis has the same lattice geometry and a similar lattice spacing.

In [7] calculations were performed with dynamical sea quarks, at a pion mass of $m_\pi = 340\text{MeV}$. I took the final tuned values they given there for the parameters as my initial guess. They can be found in the first line of table 5.

For a given value of the parameters $P = (m_0, \nu, c_{\text{sw}})$ I took different gauge field configurations as independent observations. On each I calculated the contractions for η_b and for the spin averaged $\Upsilon(1S)$. The jackknife samples of the correlators were computed with equation (66).

Note that for all values of P the same configuration and the same source points were used, resulting in reduced statistical fluctuation. I followed the tuning procedure described in subsection 2.6 to calculate the new parameters. As step size h I used $P/1000$ for the last tuning step and $P/100$ for the others. For the last tuning step $h = P/1000$ was chosen, because the previous tuning step was an interpolation, and hence a fur-

ther tuning step at $h = P/100$ was not expected to meaningfully increase precision. The experimental values $m_{\eta_b} = 9389.7\text{MeV}$ and the splitting $m_{\Upsilon(1S)} - m_{\eta_b} = 62.3\text{MeV}$ were taken from [2]. The experimental equivalent of $c_{\eta_b}^2$ is the squared speed of light with a value of 1.

In table 5 I present the values and the jackknife errors of the parameters for each tuning step. The 5th tuning step was the final tuning step.

Therefore, the optimal parameters P_{opt} are $c_{\text{sw}} = 10.135 \pm 0.051$, $\nu = 3.6882 \pm 0.0074$ and $m_0 = 8.767 \pm 0.017$.

With the given step sizes, the 4th tuning step was an interpolation, hence, the tuning could have been stopped there. For the last step the step size was reduced by approximately a factor of 10. In table 3 I introduced the quantity ΔP as how much the

Table 3: $\sigma_P/\Delta P$ for each tuning step.

Step	$\frac{\sigma_{c_{\text{sw}}}}{\Delta c_{\text{sw}}}$	$\frac{\sigma_{\nu}}{\Delta \nu}$	$\frac{\sigma_{m_0}}{\Delta m_0}$
1	0.014	0.053	0.019
2	-0.077	1.6	0.094
3	-1.2	-2.9	1.7
4	-227	-75	191

parameters changed in the current tuning step. For each tuning step I repor the ratio $\left| \frac{\sigma_i}{\Delta P_i} \right|$. Large values of $\left| \frac{\sigma_i}{\Delta P_i} \right|$ compared to 1 indicate that the tuning step is dominated by noise and small values indicate, that noise is negligible.

One can see, that for the first two tuning steps noise is negligible. For the third tuning step the effects of the noise were on the same scale as the change of parameters.

For the 4th tuning step the noise was dominant, and therefore no meaningful improvement should be expected. Table 4 supports this. For the first 3 tuning steps all the observables change by at least their jackknife error. For the 4th tuning step none of them do. I conclude, that the last tuning step could have been skipped.

In table 4 I show the values of m_{η_b} , $m_{\Upsilon(1S)} - m_{\eta_b}$ and $c_{\eta_b}^2$ calculated on the lattice, for every tuning step. These observables seem to converge towards their experimental values. After the third tuning step they were within bounds of error compatible with the experimental values. This further supports, that the tuning could have been stopped after the third tuning step.

With the last tuning step the mass of η_b further improved and the splitting changed

insignificantly. However, $c_{\eta_b}^2$ increased minimally. This may have been the result of the decreased step size used for the last tuning step.

Finally, I note that optimizing the number of samples used for each tuning step is a nontrivial task. The tuning algorithm described in section 2.6 does generally not converge within a single iteration for two reasons. The function $F(P)$ (see section 2.6) is non-linear and the local estimates of its partial derivatives have finite statistical uncertainties which decreases with increased statistics. It may be an interesting question for a follow-up work, to determine how to optimize the number of samples used for a given tuning step, such that the total usage of computational resources for the tuning process is minimized.

Table 4: Measured observables for each tuning step and experimental masses according to [2].

Step	$m_{\eta_b}[\text{MeV}]$	$m_{\Upsilon(1S)} - m_{\eta_b}[\text{MeV}]$	$c_{\eta_b}^2$
1	9161.14 ± 0.88	23.83 ± 0.22	0.8397 ± 0.0032
2	9255.89 ± 0.89	72.07 ± 0.61	1.0556 ± 0.0043
3	9391.61 ± 0.88	62.84 ± 0.54	1.0042 ± 0.0041
4	9398.68 ± 0.88	62.30 ± 0.53	1.0001 ± 0.0041
5	9398.70 ± 0.88	62.30 ± 0.53	1.0009 ± 0.0040
experimental	9398.70 ± 2.0	62.3 ± 3.2	1

Table 5: Tuned action parameters for each tuning step.

Step	c_{sw}	ν	m_0
1	4.9625	3.1918	7.3258
2	10.838 ± 0.081	3.686 ± 0.026	8.584 ± 0.024
3	10.181 ± 0.050	3.6917 ± 0.0096	8.757 ± 0.016
4	10.135 ± 0.053	3.6883 ± 0.0098	8.767 ± 0.016
5	10.135 ± 0.051	3.6882 ± 0.0074	8.767 ± 0.017

4 Conclusion

In this thesis, I implemented a numerical algorithm in which the RHQ action is used to extract energies of low-lying quarkonium states. Using this I non-perturbatively tuned the free parameters of this action with experimental data for the quarkonium spectrum. I demonstrated that this setup can be used to tune heavy-quark actions up to high precision.

I established a framework that can serve as a basis for future calculations of highly excited mesonic states and exotic mesons from first principles in lattice QCD.

Within the research group of Marc Wagner, in parallel to this thesis a M.Sc. student is attempting to construct a formalism, with which the description of radially and orbitally excited hadrons could be improved. Should that project yield favorable results, the formalism could be used to improve the accuracy of calculations of such orbitally excited states.

In parallel to this a Ph.D. student is using BOEFT for which accurate lattice data of exotic or highly excited mesonic states would yield constraints. Follow-up work on this bachelor thesis could provide such data.

Acknowledgements

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5 Appendix

5.1 Statistical methods

In this thesis I use the jackknife method, to estimate statistical uncertainties, and to calculate the mean, of observables on the lattice as well as for derived quantities. Assuming one has N independent observations of a vector $X^{(k)}$ $k = 1, 2, \dots, N$, and on a single observation a value $f(X^{(k)})$ can be calculated, then

$$X_J^{(k)} := \frac{1}{N-1} \sum_{n \neq k} X^{(n)} \quad (66)$$

defines the k th jackknife sample and $f_J^{(k)} := f(X_J^{(k)})$ is set to be the value f takes on the k -th jackknife sample. The jackknife mean $\overline{f_J}$ is given as:

$$\overline{f_J} := \frac{1}{N} \sum_k f_J^{(k)} \quad (67)$$

and the jackknife Variance s_J^2 :

$$s_J^2 := \overline{f_J^2} - \overline{f_J}^2 \quad (68)$$

where

$$\overline{f_J^2} := \frac{1}{N} \sum_n \left(f_J^{(n)} \right)^2. \quad (69)$$

Finally the jackknife estimate for the standard deviation is

$$\sigma_J = s_J \sqrt{N-1}. \quad (70)$$

. I also call σ_J the jackknife error. The jackknife covariance matrix cov_J is defined as

$$\text{cov}_J = \frac{N-1}{N} \sum_{k=1}^N \left(X_J^{(k)} - \overline{X_J} \right) \left(X_J^{(k)} - \overline{X_J} \right)^\top \quad (71)$$

where $\overline{X_J}$ is the mean. For more detailed discussion of the jackknife method see [14] and for a pedagogical introduction see [15].

In this thesis, independent observations $X^{(k)}$ are approximately uncorrelated gauge field configurations. Values are reported as jackknife mean $\pm 1\sigma_J$.

5.2 Spectral decomposition of quarkonium correlators on the periodic lattice

Here I show how the spectral decomposition of a quarkonium correlator in momentum space can be calculated on the periodic lattice.

On the periodic lattice, with temporal extent $\beta := N_t$ the expectation value of an observable $\mathcal{A}$ is:

$$\langle \mathcal{A}(t) \rangle = \frac{1}{Z} \text{Tr} \{ e^{-\beta H} \mathcal{A}(t) \} \quad (72)$$

with

$$Z = \text{Tr} \{ e^{-\beta H} \}. \quad (73)$$

Let $\{|n\rangle\}, n = \Omega, 0, 1, \dots$ be a complete set of energy eigenstates of the QCD Hamiltonian H , with $H|n\rangle = E_n|n\rangle$, where $|\Omega\rangle$ is the vacuum state.

Since for QCD $[H, P] = [H, \hat{p}] = 0$ where $\hat{p}$ is the impulse operator, the $|n\rangle$ can be chosen to also be momentum eigenstates. I therefore write $|n\rangle = |\vec{k}_n, s_n\rangle$ where s_n represents quantum numbers, whose operators commute with Parity. I choose a normalization with $\langle n'|n\rangle = \langle \vec{k}_{n'}, s_{n'} | \vec{k}_n, s_n \rangle = \delta_{\vec{k}_n, \vec{k}_{n'}} \delta_{s_n, s_{n'}}$. Substituting $\mathcal{A}(t) = \bar{\mathcal{O}}_Q(\vec{p}, t) \mathcal{O}_Q(\vec{p}, 0)$, $1 = \sum_n |n\rangle \langle n|$ and $\mathcal{A}(t) = e^{Ht} \mathcal{A}(0) e^{-Ht}$ into equation (72) and defining $\tilde{\mathcal{O}}_Q(\vec{p}) := \bar{\mathcal{O}}_Q(\vec{p}, 0)$ yields:

$$C(\vec{p}, t) = \langle \tilde{\mathcal{O}}_Q(\vec{p}, t) \tilde{\mathcal{O}}_Q^\dagger(\vec{p}, 0) \rangle = \frac{\text{Tr} [e^{-\beta H} e^{Ht} \tilde{\mathcal{O}}_Q(\vec{p}) e^{-Ht} \tilde{\mathcal{O}}_Q^\dagger(\vec{p})]}{Z} \quad (74)$$

$$= \frac{1}{Z} \sum_m \left\langle m \left| e^{-\beta H} e^{Ht} \tilde{\mathcal{O}}_Q(\vec{p}) \sum_n |n\rangle \langle n| e^{-Ht} \tilde{\mathcal{O}}_Q^\dagger(\vec{p}) \right| m \right\rangle \quad (75)$$

$$= \frac{1}{Z} \sum_{m,n} e^{-\beta E_m} e^{E_m t} e^{-E_n t} \langle m | \tilde{\mathcal{O}}_Q(\vec{p}) | n \rangle \langle n | \tilde{\mathcal{O}}_Q^\dagger(\vec{p}) | m \rangle \quad (76)$$

$$= \frac{1}{Z} \sum_{m,n} e^{-\beta E_m} e^{E_m t} e^{-E_n t} A_{mn}. \quad (77)$$

Note that $\tilde{\mathcal{O}}_Q^\dagger(\vec{p})$ increases the momentum of $|n\rangle$ by $\vec{p}$, such that

$$\langle n' | \tilde{\mathcal{O}}_Q^\dagger(\vec{p}) | n \rangle = \langle \vec{k}_{n'}, s_{n'} | \tilde{\mathcal{O}}_Q^\dagger(\vec{p}) | \vec{k}_n, s_n \rangle \delta_{\vec{k}_n + \vec{p}, \vec{k}_{n'}}. \quad (78)$$

With this, the double sum in equation (77) can be expanded as

$$C(\vec{p}, t) = \frac{1}{Z} \sum_{s_m, s_n} \sum_{\vec{k}_m, \vec{k}_n} e^{-\beta E_{s_m}(\vec{k}_m)} e^{E_{s_m}(\vec{k}_m)t} e^{-E_{s_n}(\vec{k}_n)t} \times \langle \vec{k}_m, s_m | \tilde{\mathcal{O}}_Q(\vec{p}) | \vec{k}_n, s_n \rangle \langle \vec{k}_n, s_n | \tilde{\mathcal{O}}_Q^\dagger(\vec{p}) | \vec{k}_m, s_m \rangle \delta_{\vec{k}_m + \vec{p}, \vec{k}_n} \quad (79)$$

$$= \frac{1}{Z} \sum_{s_m, s_n} \sum_{\vec{k}_m} e^{-\beta E_{s_m}(\vec{k}_m)} e^{E_{s_m}(\vec{k}_m)t} e^{-E_{s_n}(\vec{k}_m + \vec{p})t} \times \langle \vec{k}_m, s_m | \tilde{\mathcal{O}}_Q(\vec{p}) | \vec{k}_m + \vec{p}, s_n \rangle \langle \vec{k}_m + \vec{p}, s_n | \tilde{\mathcal{O}}_Q^\dagger(\vec{p}) | \vec{k}_m, s_m \rangle. \quad (80)$$

Here I define $E_{s_m}(\vec{k}_m) := E_m$ I further define the correlator in which only vacuum contributions, i.e. those with $m = \Omega$ or $n = \Omega$, are retained:

$$C_\Omega(\vec{p}, t) = \frac{1}{Z} \sum_{s_n} e^{-\beta E_\Omega(\vec{0})} e^{E_\Omega(\vec{0})t} e^{-E_{s_n}(\vec{p})t} \times \langle \vec{0}, s_\Omega | \tilde{\mathcal{O}}_Q(\vec{p}) | \vec{p}, s_n \rangle \langle \vec{p}, s_n | \tilde{\mathcal{O}}_Q^\dagger(\vec{p}) | \vec{0}, s_\Omega \rangle \quad (81)$$

$$+ \frac{1}{Z} \sum_{s_m} e^{-\beta E_{s_m}(-\vec{p})} e^{E_{s_m}(-\vec{p})t} e^{-E_\Omega(\vec{0})t} \times \langle -\vec{p}, s_m | \tilde{\mathcal{O}}_Q(\vec{p}) | \vec{0}, s_\Omega \rangle \langle \vec{0}, s_\Omega | \tilde{\mathcal{O}}_Q^\dagger(\vec{p}) | -\vec{p}, s_m \rangle. \quad (82)$$

After relabeling

$$s_m \rightarrow s, \quad s_n \rightarrow s,$$

and using

$$E_\Omega(\vec{0}) = E_\Omega, \quad E_s(\vec{p}) = E_s(-\vec{p}),$$

this becomes

$$C_\Omega(\vec{p}, t) = \frac{1}{Z} \sum_s e^{-\beta E_\Omega} e^{E_\Omega t} e^{-E_s(\vec{p})t} \langle \vec{0}, s_\Omega | \tilde{\mathcal{O}}_Q(\vec{p}) | \vec{p}, s \rangle \langle \vec{p}, s | \tilde{\mathcal{O}}_Q^\dagger(\vec{p}) | \vec{0}, s_\Omega \rangle + \frac{1}{Z} \sum_s e^{-\beta E_s(\vec{p})} e^{E_s(\vec{p})t} e^{-E_\Omega t} \langle -\vec{p}, s | \tilde{\mathcal{O}}_Q(\vec{p}) | \vec{0}, s_\Omega \rangle \langle \vec{0}, s_\Omega | \tilde{\mathcal{O}}_Q^\dagger(\vec{p}) | -\vec{p}, s \rangle. \quad (83)$$

Using the equality

$$\left| \langle \vec{p}, s_m | \tilde{\mathcal{O}}^\dagger(\vec{p}) | \vec{0}, s_\Omega \rangle \right|^2 = \left| \langle \vec{0}, s_\Omega | \tilde{\mathcal{O}}^\dagger(\vec{p}) | -\vec{p}, s_m \rangle \right|^2 \quad (84)$$

proven in section 5.3.

Defining the overlap factor

$$A_{\Omega s}(\vec{p}) := \langle \vec{0}, s_{\Omega} | \tilde{\mathcal{O}}_Q(\vec{p}) | \vec{p}, s \rangle \langle \vec{p}, s | \tilde{\mathcal{O}}_Q^{\dagger}(\vec{p}) | \vec{0}, s_{\Omega} \rangle, \quad (85)$$

I obtain

$$C_{\Omega}(\vec{p}, t) = \frac{1}{Z} \sum_s \left(e^{-\beta E_{\Omega}} e^{E_{\Omega} t} e^{-E_s(\vec{p}) t} + e^{-\beta E_s(\vec{p})} e^{E_s(\vec{p}) t} e^{-E_{\Omega} t} \right) A_{\Omega s}(\vec{p}) \quad (86)$$

$$= \frac{2}{Z} \sum_s A_{\Omega s}(\vec{p}) e^{-\frac{\beta}{2}(E_s(\vec{p}) + E_{\Omega})} \cosh \left[(E_s(\vec{p}) - E_{\Omega}) \left(t - \frac{\beta}{2} \right) \right]. \quad (87)$$

I set $p := |\vec{p}|$ and N_p as the number of vectors $\vec{p}$ with $|\vec{p}| = p$ that can be realized on the lattice. The dispersion relation (51) can be reparametrized by $E_s(p) := \frac{1}{N_p} \sum_{|\vec{p}|=p} E_s(\vec{p})$ as $E(\vec{p})$ only depend on the amplitude of $\vec{p}$. I define $A_{\Omega s}(p) := \frac{1}{N_p} \sum_{|\vec{p}|=p} A_{\Omega s}(\vec{p})$ and

$$C_{\Omega}(p, t) := \frac{1}{N_p} \sum_{|\vec{p}|=p} C_{\Omega}(\vec{p}, t) = \frac{2}{Z} \sum_s A_{\Omega s}(p) e^{-\frac{\beta}{2}(E_s(p) + E_{\Omega})} \cosh \left[(E_s(p) - E_{\Omega}) \left(t - \frac{\beta}{2} \right) \right]. \quad (88)$$

I define $s = 0$ to be the ground state with nonzero $A_{\Omega s}(p)$. The corresponding term dominates $C_{\Omega}(p, t)$ sufficiently far away from $t = 0$ and $t = N_T$. With this follows

$$C_{\Omega}(p, t) \approx \frac{2}{Z} A_{\Omega 0}(p) e^{-\frac{\beta}{2}(E_0(p) + E_{\Omega})} \cosh \left[(E_0(p) - E_{\Omega}) \left(t - \frac{\beta}{2} \right) \right]. \quad (89)$$

5.3 Proof of matrix element equality

First I need some properties of $\mathcal{O}_Q(\vec{p})$.

From equation (34) I can read off

$$\mathcal{O}_Q^{\dagger}(\vec{n}) = -\eta_{\Gamma} \mathcal{O}_Q(\vec{n}),$$

From equation (43) $\mathcal{O}_Q^{\dagger}(\vec{p}, t)$ follows as:

$$\mathcal{O}_Q^{\dagger}(\vec{p}, t) = \frac{1}{\sqrt{|\Lambda_3|}} \sum_{\vec{n}} e^{+i\vec{p} \cdot \vec{n}} \mathcal{O}_Q^{\dagger}(\vec{n}, t).$$

$$\begin{aligned}
P^{-1}\tilde{\mathcal{O}}_Q^\dagger(\vec{p}, t)P &= P^{-1}\frac{1}{\sqrt{|\Lambda_3|}}\sum_{\vec{n}}e^{+i\vec{p}\cdot\vec{n}}\mathcal{O}_Q^\dagger(\vec{n}, t)P \\
&= \pm\frac{1}{\sqrt{|\Lambda_3|}}\sum_{\vec{n}}e^{+i\vec{p}\cdot\vec{n}}\mathcal{O}_Q^\dagger(-\vec{n}, t) = \pm\frac{1}{\sqrt{|\Lambda_3|}}\sum_{\vec{m}}e^{-i\vec{p}\cdot\vec{m}}\mathcal{O}_Q^\dagger(\vec{m}, t) \\
&= \pm\tilde{\mathcal{O}}_Q^\dagger(-\vec{p}, t)
\end{aligned} \tag{90}$$

For $t = 0$ I set $\tilde{\mathcal{O}}_Q^\dagger(\vec{p}) := \tilde{\mathcal{O}}_Q^\dagger(\vec{p}, 0)$ and $\tilde{\mathcal{O}}_Q(\vec{p}) := \tilde{\mathcal{O}}_Q(\vec{p}, 0)$.

Using this, I find

$$P^{-1}\tilde{\mathcal{O}}_Q^\dagger(\vec{p})P = \pm\tilde{\mathcal{O}}_Q^\dagger(-\vec{p}). \tag{91}$$

Now I prove equation (84).

I can use that for arbitrary states $\langle\psi|$, $|\phi\rangle$ and a linear operator A $\langle\phi|A|\psi\rangle = \langle\psi|A^\dagger|\phi\rangle^*$ where $*$ denotes complex conjugation. With this I find

$$\begin{aligned}
\left(\langle\vec{p}, s_m|\tilde{\mathcal{O}}_Q^\dagger(\vec{p})|\vec{0}, s_\Omega\rangle\right)^* &= \langle\vec{0}, s_\Omega|\tilde{\mathcal{O}}_Q(\vec{p})|\vec{p}, s_m\rangle \\
&= \langle\vec{0}, s_\Omega|P(P^{-1}\tilde{\mathcal{O}}_Q(\vec{p})P)P^{-1}|\vec{p}, s_m\rangle \\
&= \pm\eta_{s_m}\langle\vec{0}, s_\Omega|\tilde{\mathcal{O}}_Q^\dagger(\vec{p})|-\vec{p}, s_m\rangle,
\end{aligned} \tag{92}$$

where $P^{-1}|\vec{p}, s_m\rangle = \eta_{s_m}|-\vec{p}, s_m\rangle$ with $|\eta_{s_m}| = 1$ and $\langle\vec{0}, s_\Omega|P = \langle\vec{0}, s_\Omega|$ were used. Therefore

$$\left|\langle\vec{p}, s|\tilde{\mathcal{O}}_Q^\dagger(\vec{p})|\vec{0}, s_\Omega\rangle\right|^2 = \left|\langle\vec{0}, s_\Omega|\tilde{\mathcal{O}}_Q^\dagger(\vec{p})|-\vec{p}, s\rangle\right|^2$$

holds, which concludes the proof.

5.4 γ_5 hermiticity proof

In this section I will prove, that the Dirac operator D_{RHQ} satisfies equation (41). From equation (12) it can be read off as

$$D_{\text{RHQ}} = A_1 + A_2 + A_3 + A_4 \tag{93}$$

where A_1, A_2, A_3 and A_4

$$A_1 = m_0, \quad (94)$$

$$A_2 = \gamma_4 D_4 + \nu \gamma_i D_i, \quad (95)$$

$$A_3 = -\frac{a}{2} D_4^2 - \frac{a}{2} \nu (D_i D_i), \quad (96)$$

$$A_4 = \sum_{\mu, \nu} \frac{ia}{4} c_{\text{sw}} \sigma_{\mu\nu} F_{\mu\nu}. \quad (97)$$

. First, I rewrite the covariant derivative D_μ in its matrix representation.

$$D_{\mu, nm}^{ab} = \frac{1}{2a} \left[U_\mu^{ab}(n) \delta_{n+\hat{\mu}, m} - (U_\mu^{ab})^\dagger(n - \hat{\mu}) \delta_{n-\hat{\mu}, m} \right] \quad (98)$$

$$(D_{\mu, nm}^{ab})^\dagger = \frac{1}{2a} \left[U_\mu^{ab}(n) \delta_{n+\hat{\mu}, m} - (U_\mu^{ab})^\dagger(n - \hat{\mu}) \delta_{n-\hat{\mu}, m} \right]^\dagger \quad (99)$$

$$= \frac{1}{2a} \left[(U_\mu^{ab})^\dagger(m) \delta_{m+\hat{\mu}, n} - U_\mu^{ab}(m - \hat{\mu}) \delta_{m-\hat{\mu}, n} \right] \quad (100)$$

$$= -\frac{1}{2a} \left[U_\mu^{ab}(m - \hat{\mu}) \delta_{m-\hat{\mu}, n} - (U_\mu^{ab})^\dagger(m) \delta_{m+\hat{\mu}, n} \right] \quad (101)$$

$$= -\frac{1}{2a} \left[U_\mu^{ab}(n) \delta_{m, n+\hat{\mu}} - (U_\mu^{ab})^\dagger(n - \hat{\mu}) \delta_{m, n-\hat{\mu}} \right] \quad (102)$$

$$= -D_{\mu, nm}^{ab}. \quad (103)$$

I can finally write

$$D_\mu^\dagger = -D_\mu \quad (104)$$

and

$$(D_\mu^2)^\dagger = (D_\mu D_\mu)^\dagger = (D_\mu^\dagger)^2 = D_\mu^2. \quad (105)$$

With $F_{\mu\nu}^\dagger = -F_{\mu\nu}$ and $\sigma_{\mu\nu}^\dagger = \sigma_{\mu\nu}$ and equations (94)-(97) it follows that

$$A_1^\dagger = A_1, \quad (106)$$

$$A_2^\dagger = -A_2, \quad (107)$$

$$A_3^\dagger = A_3, \quad (108)$$

$$A_4^\dagger = A_4. \quad (109)$$

With $[\gamma_5, D_\mu] = [\gamma_5, \sigma_{\mu\nu}] = 0$ and $\{\gamma_5, \gamma_\mu\} = 0$ it further follows:

$$\gamma_5 A_1 \gamma_5 = A_1, \quad (110)$$

$$\gamma_5 A_2 \gamma_5 = -A_2, \quad (111)$$

$$\gamma_5 A_3 \gamma_5 = A_3, \quad (112)$$

$$\gamma_5 A_4 \gamma_5 = A_4. \quad (113)$$

Comparing equations (106) - (113) yields $D_{\text{RHQ}}^\dagger = \gamma_5 D_{\text{RHQ}} \gamma_5$ which completes the proof of the γ_5 hermiticity of D_{RHQ}

References

- [1] C. E. Thomas, “Meson Spectroscopy from Lattice QCD,” *Few Body Syst.* **58** no. 3, (2017) 122.
- [2] **Particle Data Group** Collaboration, S. Navas *et al.*, “Review of particle physics,” *Phys. Rev. D* **110** no. 3, (2024) 030001.
- [3] M. Wagner, “Spectroscopy of heavy exotic mesons using lattice qcd static potentials and the born-oppenheimer approximation.” 2023. <https://arxiv.org/abs/2308.04530>.
- [4] M. Berwein, N. Brambilla, A. Mohapatra, and A. Vairo, “Hybrids, tetraquarks, pentaquarks, doubly heavy baryons, and quarkonia in Born-Oppenheimer effective theory,” *Phys. Rev. D* **110** no. 9, (2024) 094040, [arXiv:2408.04719](https://arxiv.org/abs/2408.04719) [[hep-ph](#)].
- [5] M. Wagner, S. Diehl, T. Kuske, and J. Weber, “An introduction to lattice hadron spectroscopy for students without quantum field theoretical background,” 10, 2013. [arXiv:1310.1760](https://arxiv.org/abs/1310.1760) [[hep-lat](#)].
- [6] S. Aoki, Y. Kuramashi, and S.-i. Tominaga, “Relativistic heavy quarks on the lattice,” *Prog. Theor. Phys.* **109** (2003) 383–413, [arXiv:hep-lat/0107009](https://arxiv.org/abs/hep-lat/0107009).
- [7] **RBC, UKQCD** Collaboration, Y. Aoki, N. H. Christ, J. M. Flynn, T. Izubuchi, C. Lehner, M. Li, H. Peng, A. Soni, R. S. Van de Water, and O. Witzel, “Nonperturbative tuning of an improved relativistic heavy-quark action with application to bottom spectroscopy,” *Phys. Rev. D* **86** (2012) 116003, [arXiv:1206.2554](https://arxiv.org/abs/1206.2554) [[hep-lat](#)].

- [8] C. Gattringer and C. B. Lang, *Quantum chromodynamics on the lattice*, vol. 788. Springer, Berlin, 2010.
- [9] M. Guagnelli, R. Sommer, and H. Wittig, “Precision computation of a low-energy reference scale in quenched lattice qcd,” *Nuclear Physics B* **535** no. 1-2, (Dec., 1998) 389–402.
[http://dx.doi.org/10.1016/S0550-3213\(98\)00599-9](http://dx.doi.org/10.1016/S0550-3213(98)00599-9).
- [10] R. Sommer, “A new way to set the energy scale in lattice gauge theories and its application to the static force and σ_s in su (2) yang-mills theory,” *Nuclear Physics B* **411** no. 2-3, (Jan., 1994) 839–854.
[http://dx.doi.org/10.1016/0550-3213\(94\)90473-1](http://dx.doi.org/10.1016/0550-3213(94)90473-1).
- [11] C. Lehner, “Grid python toolkit (gpt),” <https://github.com/lehner/gpt>, 2026. Accessed: 2026-06-23.
- [12] P. Boyle, A. Yamaguchi, G. Cossu, and A. Portelli, “Grid: A next generation data parallel c++ qcd library,” *PoS LATTICE2015* (2016) 023, [arXiv:1512.03487](https://arxiv.org/abs/1512.03487) [[hep-lat](#)].
- [13] S. Meinel, “Status of next-generation $\Lambda_b \rightarrow p, \Lambda, \Lambda_c$ form-factor calculations,” *PoS LATTICE2023* (2024) 275, [arXiv:2309.01821](https://arxiv.org/abs/2309.01821) [[hep-lat](#)].
- [14] F. G. Mohammad and W. J. Percival, “Creating jackknife and bootstrap estimates of the covariance matrix for the two-point correlation function,” *Mon. Not. Roy. Astron. Soc.* **514** no. 1, (2022) 1289–1301, [arXiv:2109.07071](https://arxiv.org/abs/2109.07071) [[astro-ph.CO](#)].
- [15] P. Young, “Everything you wanted to know about data analysis and fitting but were afraid to ask.” 2014. <https://arxiv.org/abs/1210.3781>.